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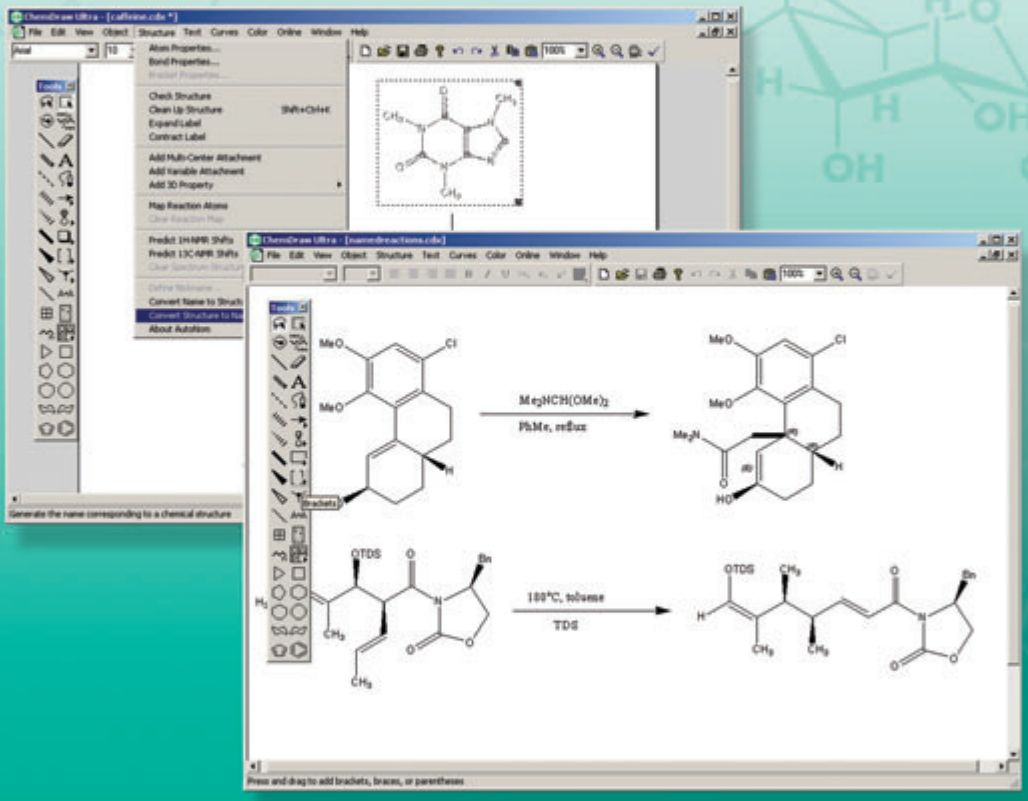

ChemDraw®

Chemical Structure Drawing Standard

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User's Guide

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CS ChemDraw 9.0

for Windows and Macintosh

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ChemDraw®

Chemical Structure Drawing Standard

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Q: That makes sense, but what do I get out of purchasing my own software?

A: When you purchase authorized copies of software programs, you receive user guides and tutorials, quick reference cards, the opportunity to purchase upgrades, and technical support from the software publishers. For most software programs, you can read about user benefits in the registration brochure or upgrade flyer in the product box.

Q: What exactly does the law say about copying software?

A: The law says that anyone who purchases a copy of software has the right to load that copy onto a single computer and to make another copy "for archival purposes only" or, in limited circumstances, for "purposes only of maintenance or repair." It is illegal to use that software on more than one computer or to make or distribute copies of that software for any other purpose unless specific permission has been obtained from the copyright owner. If you pirate software, you may face not only a civil suit for damages and other relief, but criminal liability as well, including fines and jail terms of up to one year

Q: So I'm never allowed to copy software for any other reason?

A: That's correct. Other than copying the software you purchase onto a single computer and making another copy "for archival purposes only" or "purposes only of maintenance or repair," the copyright law prohibits you from making additional copies of the software for any other reason unless you obtain the permission of the software company.

Q: At my company, we pass disks around all the time. We all assume that this must be okay since it was the company that purchased the software in the first place.

A: Many employees don't realize that corporations are bound by the copyright laws, just like everyone else. Such conduct exposes the company (and possibly the persons involved) to liability for copyright infringement. Consequently, more and more corporations concerned about their liability have written policies against such "softlifting". Employees may face disciplinary action if they make extra copies of the company's software for use at home or on additional computers within the office. A good rule to remember is that there must be one authorized copy of a software product for every computer upon which it is run

Q: Can I take a piece of software owned by my company and install it on my personal computer at home if instructed by my supervisor?

A: A good rule of thumb to follow is one software package per computer, unless the terms of the license agreement allow for multiple use of the program. But some software publishers' licenses allow for "remote" or "home" use of their software. If you travel or telecommute, you may be permitted to copy your software onto a second machine for use when you are not at your office computer. Check the license carefully to see if you are allowed to do this.

Q: What should I do if become aware of a company that is not compliant with the copyright law or its software licenses?

A: Cases of retail, corporate and Internet piracy or non-compliance with software licenses can be reported on the Internet at http://www.siia.net/piracy/report.asp or by calling the Anti-Piracy Hotline: (800) 388-7478.

Q: Do the same rules apply to bulletin boards and user groups? I always thought that the reason they got together was to share software.

A: Yes. Bulletin boards and user groups are bound by the copyright law just as individuals and corporations. However, to the extent they offer shareware or public domain software, this is a perfectly acceptable practice. Similarly, some software companies offer bulletin boards and user groups special demonstration versions of their products, which in some instances may be copied. In any event, it is the responsibility of the bulletin board operator or user group to respect copyright law and to ensure that it is not used as a vehicle for unauthorized copying or distribution.

Q: I'll bet most of the people who copy software don't even know that they're breaking the law.

A: Because the software industry is relatively new, and because copying software is so easy, many people are either unaware of the laws governing software use or choose to ignore them. It is the responsibility of each and every software user to understand and adhere to copyright law. Ignorance of the law is no excuse. If you are part of an organization, see what you an do to initiate a policy statement that everyone respects. Also, suggest that your management consider conducting a software audit. Finally, as an individual, help spread the word that users should be "software legal."

Q: What are the penalties for copyright infringement?

A: The Copyright Act allows a copyright owner to recover monetary damages measured either by: (1) its actual damages plus any additional profits of the infringer attributable to the infringement, or (2) statutory damages, of up to $150,000 for each copyrighted work infringed. The copyright owner also has the right to permanently enjoin an infringer from engaging in further infringing activities and may be awarded costs and attorneys' fees. The law also permits destruction or other reasonable disposition of all infringing copies and devices by which infringing copies have been made or used in violation of the copyright owner's exclusive rights. In cases of willful infringement, criminal penalties may also be assessed against the infringer.

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"Don't Copy that Floppy" video
This 9 minute rap video, available for $10, is designed to educate students on the ethical use of software.

Other education materials including, "Software Use and the Law", a brochure detailing the copyright law and how software should be used by educational institutions, corporations and individuals; and several posters to help emphasize the message that unauthorized copying of software is illegal.

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A Guide to CambridgeSoft Manuals

	Includes	Manuals	ChemDraw Chemical Structure Drawing Standard	ChemOffice Chem3D, ChemFinder & E-Notebook	ChemOffice Enterprise Solutions And Databases
Software	ChemDraw		■		
	Chem3D			■	
	ChemFinder			■	
	E-Notebook Desktop			■	
	Inventory Desktop				■
	BioAssay Desktop				■
Desktop Applications	ChemDraw/Excel		■		
	ChemFinder/Office			■	
	CombiChem/Excel			■	
	ChemSAR/Excel			■	
	MOPAC, MM2			■	
	CS Gaussian, GAMESS Interface			■	
Enterprise Solutions	ChemOffice WebServer				■
	Oracle Cartridge				■
	E-Notebook Workgroup, Enterprise			■	
	Document Manager				■
	Registration Enterprise				■
	Formulations & Mixtures				■
	Inventory Workgroup, Enterprise				■
	Discovery LIMS				■
	BioAssay Workgroup, Enterprise				■
	BioSAR Enterprise				■
	ChemDraw/Spotfire				■
Databases	The Merck Index				■
	ChemACX, ChemSCX				■
	ChemMSDX				■
	ChemINDEX, NCI & AIDS				■
	ChemRXN				■
	Ashgate Drugs				■
Tips	Structure Drawing Tips		■		
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Introduction

About ChemDraw®

ChemDraw is a tool to enable professional scientists, science students, and scientific authors to communicate chemical structures. It is designed to work according to conventions we found most intuitive for such users. Our goal has been to make ChemDraw as easy to use as possible while providing superior drawing quality.

What's New in ChemDraw 9.0

ChemDraw 9.0 is enhanced by the following features:

- **Improved Struct=Name**. Significant improvements to the add-on that generates systematic names for chemical structures. Now with auto-update. See "Struct=Name" on page 73.
- **Improved Proton NMR predictions**. Improved display and accuracy. See "NMR Shift Information—ChemNMR" on page 147.
- **Improved TLC Plate tool**. Includes support for crescent-shaped spots, custom spots, and transparent backgrounds. See "The TLC Tool" on page 105.
- **Fragmentation tools**. The Mass Fragmentation tool is quicker and smoother. New Dissociation and Retrosynthesis tools. See "Mass Fragmentation Tool" on page 143 and "Drawing Reactions" on page 144.
- **Support for more file formats.** Import JPEG; import and export GIF, TIFF, PNG, and BMP. Import and export Chemical Markup Language (CML).
- **Expand generic structures.** Generate collections of up to 500 molecules with the expansion tool. See "Expand Generic Structures" on page 145.
- **Smarter chemical warnings**. Support for linear atoms and hydrogen bonds. Easier to use—warnings now appear on tooltips.
- **tPSA Calculation**. An algorithm to calculate Topological Polar Surface Areas for the prediction of pharmaceutical transport properties has been added to ChemProp. See "Topological Polar Surface Area" on page 246.
- **Multiple ChemDraw Items folders**. See About This User's Guide

This User's Manual contains information for the ChemDraw application for Windows and Macintosh. It assumes that you are familiar with the basics of your Windows operating system. If you are not, please refer to your system manual before using the applications. Some of the material describes tasks that must be performed in conjuction with other integrated CambridgeSoft products. The material on the Addins describes tasks that must be performed in conjuction with Microsoft Excel. If you are not familiar with this product, please consult the relevant User's Manual for more detailed information.

The chapters in this guide are organized by task. They are intended to help you familiarize yourself with the ChemDraw applications and start using them as quickly and efficiently as possible. New users should read the **Basics** chapter to get an overview of the product and how it works. Chapter 2 **Tutorials**, demonstrates most of the features of the application. Perform the tutorials in the order

they are presented. Experienced users can skip to **Chapter 3** and the subsequent chapters, which provide more detailed information.

Conventions

The following notations are used throughout this user's guide:

Ultra The Ultra symbol indicates that a feature is available in the Ultra version only.

Pro The Pro symbol indicates that a feature is available in both the Pro and Ultra versions.

Features that are available in the Standard version are not indicated by a symbol.

NOTE: *Notes such as this are used to highlight information supplemental to the main text.*

When a shortcut key sequence is given, the Windows OS sequence is listed first, with the Macintosh OS sequence following, for example: "Use the command: Shift+Control+G or Shift+Command+G to ungroup objects." For a list of keyboard shortcuts see "Shortcuts and Hotkeys" on page 247.

A bold font is used to indicate that you are to take a particular action, for example: "From the Help Menu, choose **Help Contents**."

Additional Information

Additional sources of ChemDraw information are:

- The Quick Reference Cards.
- The Help system
- CambridgeSoft Web Pages. http://www.cambridgesoft.com/

Quick Reference Card

The ChemDraw Quick Reference Cards are located in the back of the manual. The cards provide summaries of ChemDraw Desktop Application commands and features. Because many of the instructions require knowledge of the interface elements, use the Quick Reference card as you perform the tutorials in Chapter 2: "Tutorials".

Help System

ChemDraw provides the following types of Help:

- **ChemDraw Help**. An HTML reference guide.
- **Context-sensitive Help** (Windows). Help topics related to user interface objects. To access Context sensitive Help type **Shift+F1**.
- **ToolTips**. Short descriptions of user interface objects displayed by pointing.
- **Status Bar**. The lower left corner of the GUI displays useful information as you work.

CambridgeSoft Web Pages

The following table contains the addresses of ChemDraw-related web pages.

For information about ...	Access ...
Technical Support	http://www.cambridgesoft.com/services
ChemDraw Plugin	http://products.cambridgesoft.com/ProdInfo.cfm?pid=278 http://products.cambridgesoft.com/ProdInfo.cfm?pid=279

For information about ...	Access ...
Software Developer's kit	http://sdk.cambridgesoft.com/
ActiveX control	http://sdk.cambridgesoft.com/
Purchasing CambridgeSoft products and chemicals	http://chemstore.cambridgesoft.com/

Installation and System Requirements

Before installation, see the "ReadMeFirst" and any other ReadMe documents on the installation CD-ROM.

Microsoft®Windows® Requirements

- Windows 2000 or XP.
- Microsoft® Excel add-ins require Office 2000, 2003, or XP.
- ChemDraw plugins/ActiveX® controls support Netscape® 6.2.x and 7.x, Mozilla 1.x, and Microsoft IE 5.5 SP2 and 6.x. The Chem3D ActiveX control supports IE 5.5 SP2 and 6.x *only*. There is no Chem3D plugin available.

NOTE: *Windows XP Service Pack 2 includes security features that automatically block active content. This means that by default, Internet Explorer blocks ChemDraw and Chem3D ActiveX controls. To activate them, you must choose the option to "allow blocked content" from the bar appearing under the address bar notifying you that the security settings have blocked some of the content of the page. IE does not remember this information, so you must repeat the activation each time you access the page.*
If you visit a site frequently, you can add it to the list of trusted sites in IE's security settings.

- Screen resolution must be 800 x 600 or higher.

Macintosh® Requirements

- Ignore this if it shouldn't be here. It's conditional text, and disappears when not needed. Mac®OS X 10.1.x or later.
- Plugin supports Mozilla 1.0.x to 1.2..x and Netscape 7.0.
- Screen resolution must be 800 x 600 or higher.

Site License Network Installation Instructions

If you have purchased a site license, please see the following web site for network installation instructions:

http://www.cambridgesoft.com/services/sl/

Chapter 1: ChemDraw Basics

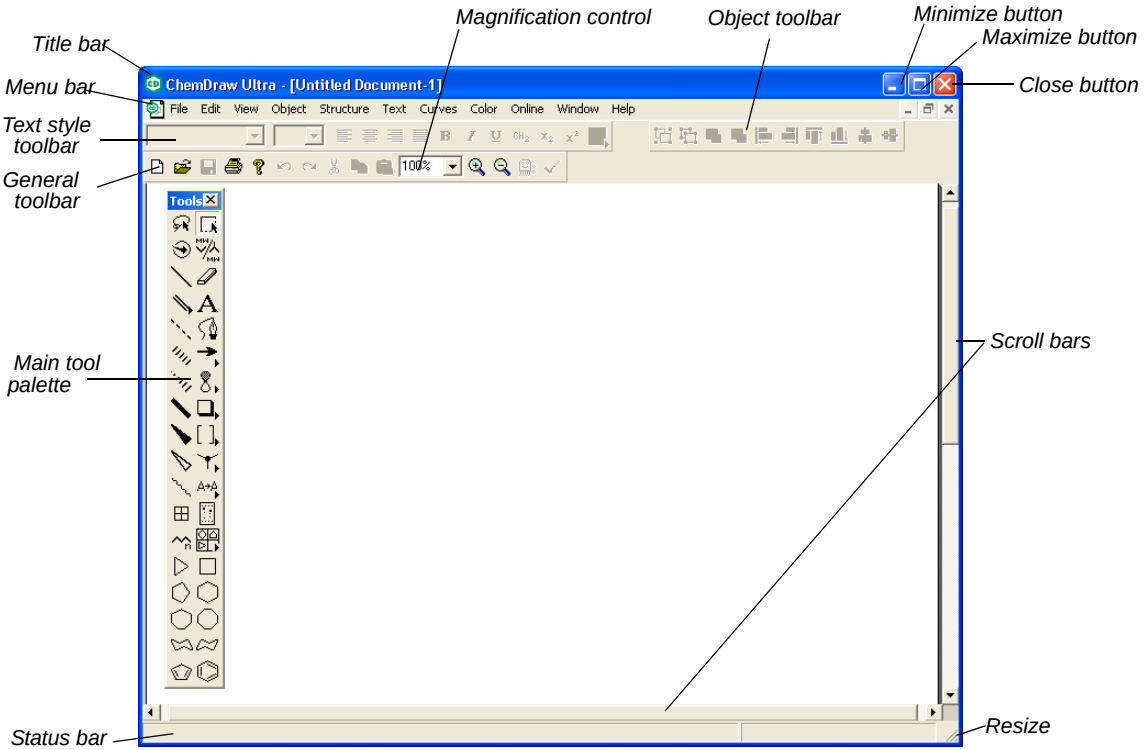
Overview

The information required to begin using ChemDraw includes how to do the following:

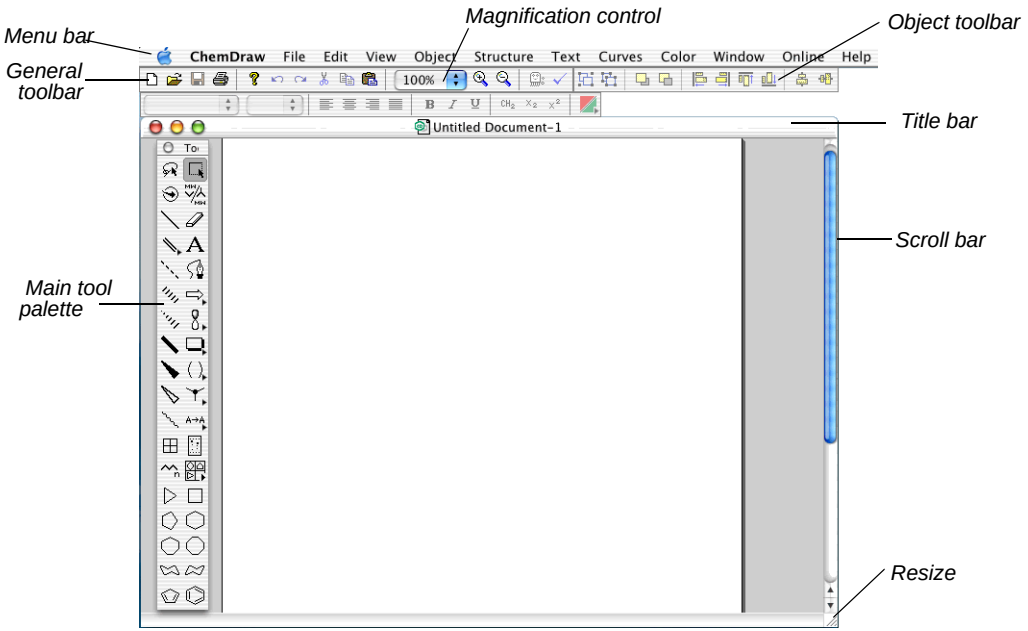
- Identify the parts of the ChemDraw interface.
- Customize parts of the user environment.
- Create, open, and save documents.
- Set printing preferences.

The ChemDraw Graphical User Interface

Although the Macintosh and Windows versions of the ChemDraw graphical user interface (GUI) differ slightly, the essential GUI consists of the same elements. The Windows version of ChemDraw is shown below.



The Mac GUI is shown below.



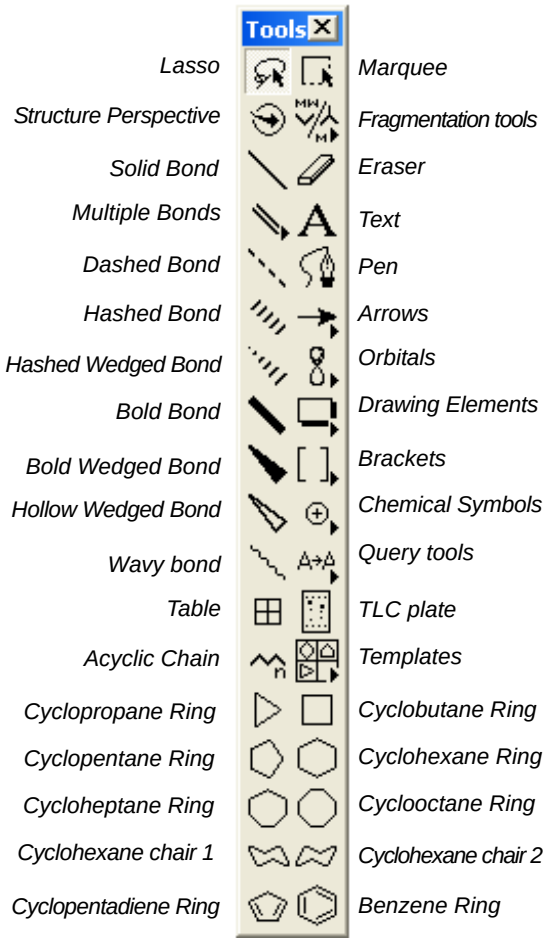
The Main Tools Palette

Use the main tools palette to create and manipulate drawings. The appearance of the toolbar is slightly different for the different versions of ChemDraw. The toolbar for ChemDraw Ultra is shown below.

The table below describes the functions of the tools for all versions. Some of the tools have multiple options that can be selected from a tool palette.

Tool	Use to...
Selection	**Lasso**. Select objects by dragging around them. **Marquee**. Select objects by dragging diagonally across them. Selected objects can be further manipulated using menu commands.
Structure Perspective	Rotate a selected object in three dimensions.
Fragmentation toolbar	**Fragmentation tool**. Splits molecules across specific bonds. **Dissociation tool**. Breaks bonds and draws a reaction. **Retrosynthesis tool**. Breaks bonds and draws a reaction.
Bond	Draw bonds and set bond properties.
Eraser	Delete objects. Click on an object to delete; drag to delete multiple objects.
Multiple Bond toolbar	Draw multiple bonds and set bond properties. Bonds of different types can be selected from the Multiple Bonds tool palette.
Text	Create atom labels and captions.
Pen	Draw freehand shapes such as custom arrows and orbitals.
Arrows toolbar	Draw arrows. Arrows of different types can be selected from the Arrows toolbar.
Orbitals toolbar	Draw orbitals. Orbitals of different types can be selected from the Orbitals toolbar.
Drawing Elements toolbar	Draw annotations that lack chemical significance, such as boxes and lines. Drawing Elements of different types can be selected from the Drawing Elements toolbar. Includes the Arc tools. ***Pro***
Brackets toolbar	Draw brackets, parentheses, and braces. Brackets of different types can be selected from the Brackets tool palette.
Chemical Symbols toolbar	Draw chemically significant symbols such as charges, radicals, and lone pairs. Symbols of different types can be selected from the Symbols tool palette.
Arcs toolbar	Draw arcs. Arcs of different degrees can be selected from the Arcs tool palette. *NOTE: The Arcs tool is a separate tool only on ChemDraw Standard.*
Acyclic Chain	Draw chains of any length.

Tool	Use to...
Query Tools toolbar	Draw stereochemical flags, indicate free sites, alternative groups and correspondences between atoms in query structures. Various options can be selected from the Query tool palette.
Templates toolbars	Draw structures with templates stored in template documents. Templates can be selected from the Templates toolbars.
Rings	Draw common structural components.
Table	Draw tables with multiple rows and columns.
TLC Plate **Pro**	Draw TLC plates with multiple lanes and adjustable solvent front and spots.



Setting the Default Tool

Use the Preferences dialog box to set which tool is automatically selected when you open documents.

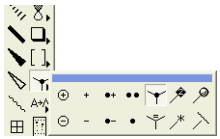
To set the default tool:

1. From the **File** menu, choose **Preferences**.
   The Preferences dialog box appears.
2. Click the **Open/Save** tab.

3. In the **Opening Files** section, click the Default Tool to be automatically selected when you open a document.

Tearing Off Palettes

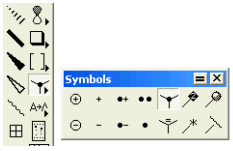
Some tools have toolbars extending from them, indicated by an arrow at the bottom right of the tool button.



You can "tear off" these toolbars and place them anywhere in the ChemDraw screen. You cannot dock torn off toolbars.

To tear off a toolbar:

- Click the arrow on the lower right of the tool.
- Holding the mouse button down, point to the title bar and release the mouse button.



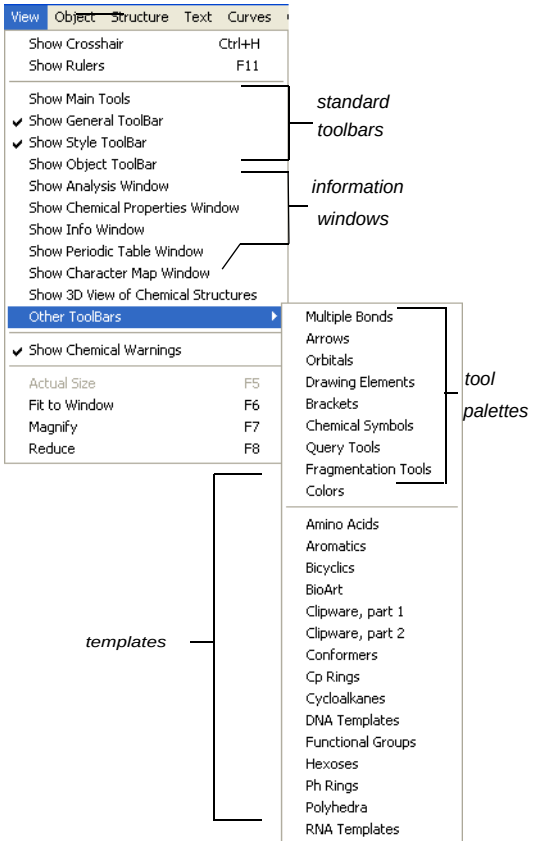
You can drag the toolbar by its title bar to reposition it.

You can also show or hide a toolbar by selecting it from the **Other Toolbars** submenu on the **View** menu.

Optional Toolbars

ChemDraw provides a number of optional toolbars and information windows to facilitate production of ChemDraw documents. These toolbars are accessed from the **View** menu. They are divided into three basic groups:

- Standard Toolbars and Show Windows
- Tool Palettes
- Templates



Showing and Hiding Toolbars

To show or hide a toolbar:

- From the **View** menu, select a toolbar.

  A check mark appears next to the item when the toolbar is displayed.

Docking and Undocking Toolbars

The standard toolbars, can be docked or undocked. Docked toolbars can attach to any edge of the

ChemDraw window. Undocked toolbars can float anywhere in the ChemDraw screen.

To dock a toolbar:

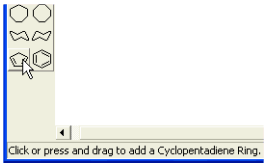
- Drag the toolbar to the edge of the ChemDraw screen where you want it to dock.
- Double-click the toolbar background. This will dock the toolbar in the default position. (All toolbars default to the top of the ChemDraw window, except for the Tools toolbar which defaults to the left side.)

To undock a toolbar:

- Drag the toolbar into the position you want.

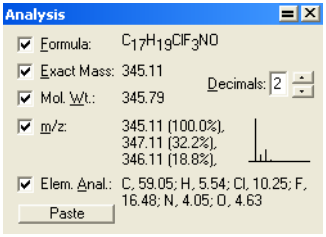
The Status Bar or Message Area (Windows)

The status bar or message area displays information about the menu or toolbar you are using.



The Analysis Window

The Analysis window displays the chemical analysis of the selected structure. If nothing is selected, the values shown are for the entire document.

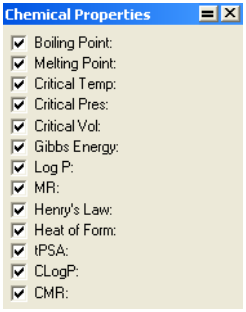


See "Viewing Analysis Information" on page 138 for information on the Analysis window.

The Paste button inserts all selected items into the document. The button shrinks the window to just the title bar.

Pro The Chemical Properties Window

The Chemical Properties window displays properties of the selected structure. When no structure is selected, properties will be displayed only if there is one (and only one) structure in the document.

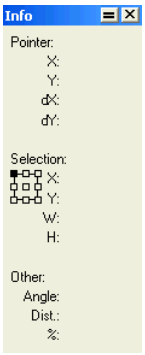


The Paste button inserts all selected items into the document. The button shrinks the window to just the title bar, while leaving it active.

NOTE: *CLogP and CMR values are displayed only in ChemDraw Ultra.*

The Info Window

The Information window shows size/positioning information about what's going on in ChemDraw.

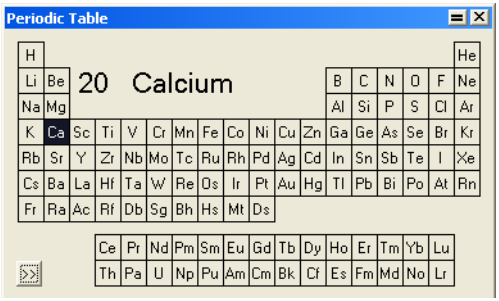


The fields show the following:

Field	Shows...
Pointer: X/Y	current mouse coordinates
Pointer: dX/dY	change in X and Y coordinates of a moved selection
Selection: X/Y	position of a selection
W/H	width/height of a selection
Angle:	angle of a bond; rotation of a selection
Dist:	length of a bond; distance a selection has been moved
%	% of original size when resizing a selection

Periodic Table

The Periodic Table window displays a floating periodic table. It can be used both for reference and to insert elements into structures.



Click an element symbol to highlight the element and activate the Text tool. Drag across the table to highlight each element in turn. Click the button to show or hide the detailed information.

After selecting an element, click in the document to add an atom label consisting of that element and the appropriate number of hydrogens. Labeling behavior is as follows:

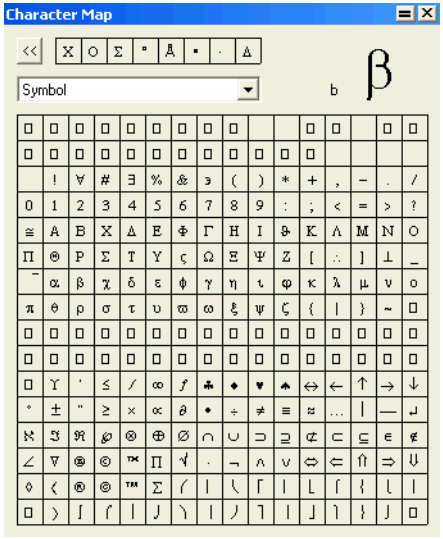
click on...	to...
an existing unlabeled atom	label the atom
an existing labeled atom	cycle the hydrogen count (if it matches the selected element) or change the label
an empty space	create a new atom

Double-clicking on an existing atom will open it for editing without changing the label.

NOTE: *Some element names conflict with ChemDraw Hotkeys, and may not be interpreted correctly by Chemical Warnings or Check Structure. For more information and troubleshooting see "Defining Nicknames" on page 122.*

Character Map

The floating Character Map window displays the 256 ASCII characters in any font. The default font is Symbol. Use it to add symbols or styled fonts to labels.‘



The character map is active only when a text box is open for editing. It will appear grayed-out at all other Times New Roman With a text box open, mouse over the character map to view a larger version of the characters in the top right corner of the window. Click any character in the table to enter that character in the text box. The selected font (shown in the character map window) is applied to that character only. It does not change the active font in the text box.

NOTE: *You can cancel a selection by dragging to some other character before releasing.*

The 8 most recently used characters are displayed at the top of the window. These characters "remember" their font and are not affected by changes to the window. A single character may appear more than once in this section if the versions use different fonts.

Click the button to toggle between the 8 most recently used characters and the entire character map.

Customizing ChemDraw

You can customize ChemDraw by configuring Preferences and Document Settings.

Preferences allow you to change the default behavior of certain options that apply to every open document. Document Settings allow you to change the default behavior of options that will affect only the active document.

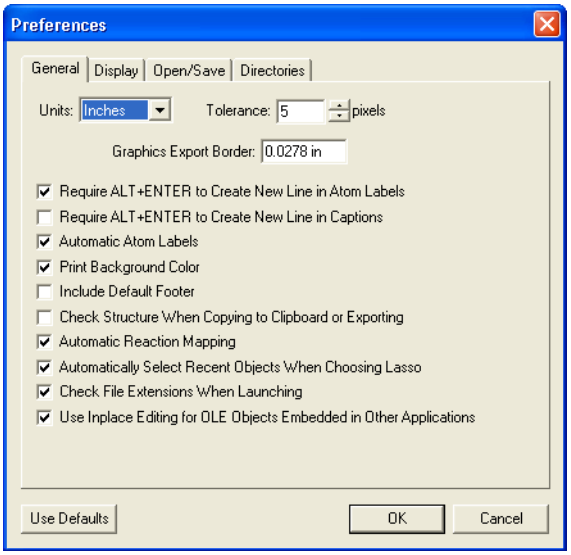
Setting Preferences

Preferences affect the way the ChemDraw application works, regardless of the document with which you are working.

To open the Preferences dialog box:

- From the **File** menu, choose **Preferences**.

The Preferences dialog box appears:



To restore the CambridgeSoft default settings:

- Click the **Use Defaults** button.

Document and Object Settings

Document and object settings are user-definable settings that are applied to the current document. Settings include:

- Drawing settings—set drawing options such as the fixed length used to draw bonds
- Caption and label text settings—set text options such as the font used for atom labels and captions
- Color settings—set available colors for objects and the document background
- Print/Page Setup—set options such as the page size used and text displayed in footers

You can apply document settings in the following ways:

- Customize settings for the entire document using the Document Settings dialog box
- Apply settings to the entire current document from an existing document
- Apply settings to selected objects in the current document from an existing document

Default Style Sheet or Stationery Pad

When you open ChemDraw, the last Style Sheet or Stationery Pad used opens as the default. If you choose another Style Sheet or Stationery Pad, that file becomes the default.

To view the default Style Sheet or Stationery Pad:

- Click the **File** menu.

  The **New** menu item displays the name of the Style Sheet or Stationery Pad.

Saving Customized Settings as Style Sheets or Stationery Pads

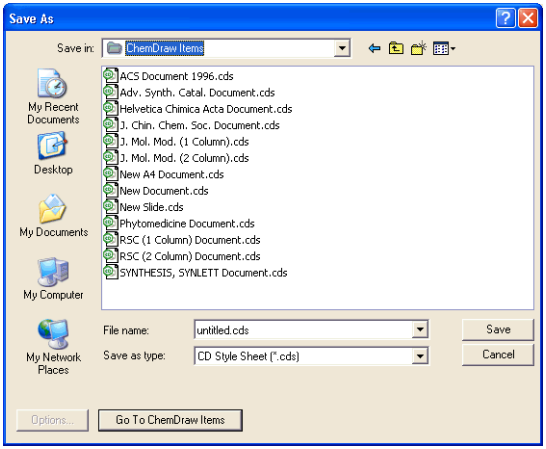
Every new document created with ChemDraw uses a Style Sheet or Stationery Pad to obtain its document settings. Style Sheets or Stationery Pads can also contain predefined objects. When you create a new document, you actually create an untitled copy of the Style Sheet or Stationery Pad. Any changes you make to the copy of the Style Sheet or Stationery Pad do not affect the Style Sheet or Stationery Pad itself.

You can create a Style Sheet or Stationery Pad with your own customized setting by saving it as a .cds file. If you store the .cds file in the ChemDraw Items folder, it appears in the **Open Special** menu so you can access it from the **File** menu.

To save a document's setting as a Style Sheet or Stationery Pad:

1. Choose **Save As** from the **File** menu.

The Save As dialog box appears.



2. Name the file and change the type (in OS X: format) to CD Style Sheet (cds) or ChemDraw Stationery.
3. To save the file in the ChemDraw items folder, click the **Go To ChemDraw Items** button.
4. Click **Save**.

Applying Document Settings From Other Documents

To apply document settings to the active window that are contained in a different document:

- On the **File** menu point to **Apply Document Settings from**, and then choose the document from which to apply the settings.

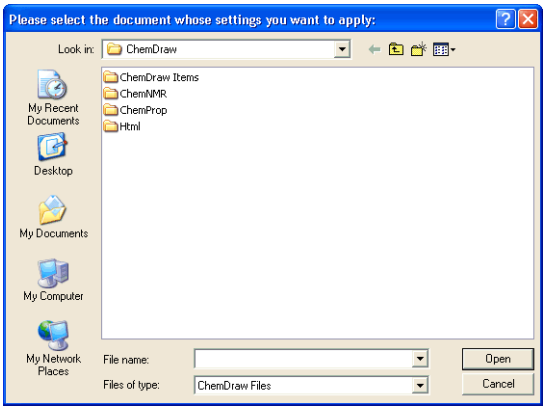
  The settings in the active document window change to those found in the Style Sheet or Stationery Pad that you choose.

NOTE: *When you apply settings, they apply to the current document only are not saved as the default for the next document. Use Open Special from the File menu if you want to change the default document settings.*

To apply the document settings from a document or style sheet not listed in the menu:

1. From the **Apply Document Settings from** submenu, choose **Other**.

   The Select document dialog box appears.



2. Open the appropriate folder and select a ChemDraw document or Style Sheet / Stationery Pad.
3. Click **Open**.

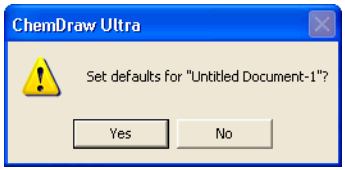
Applying Object Settings from Other Documents

You can apply settings from another document to selected objects in the current document. You can apply the chosen settings to the selected objects only, or to all new objects drawn in the current document.

To apply object settings:

1. Select the object.
2. On the **Object** menu, point to **Apply Object Settings from**, and then choose the document from which to apply the settings.

A dialog box appears:



3. Take the appropriate action:

If you want to apply the settings to the ...	Then click ...
selected object only	**No**
selected object and any new objects you draw	**Yes**

The settings are applied.

Using Documents

Documents are the ChemDraw workspace where you create and manipulate structures. You can create a new document or open an existing document and edit it.

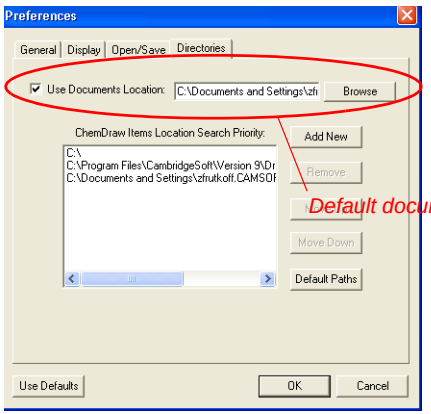
Setting the Default Document Location

You can set what file location is shown in the Open dialog box by using the Preferences dialog box.

To set the default location:

1. From the **File** menu, choose **Preferences**.

   The Preferences dialog box appears.
2. Click the **Directories** tab.
3. Click the checkbox next to **Use Documents Location** and type in or browse to the location to use.



If **Use Documents Location** is not selected, the first time you use the Open dialog box your My-Documents folder is shown. Subsequent uses show the last directory used.

Creating a Document

You can create a new, blank document using the ChemDraw default settings, or use a Style Sheet or Stationery Pad with customized settings.

Creating a New Document

To create a document:

- From the **File** menu, click **New Document**.

Creating a Document Using a Style Sheet or Stationery Pad

To create a new document using a different Style Sheet or Stationery Pad:

1. From the **File** menu, click **Open Special**.
2. Choose a **Style Sheet** or **Stationery Pad** from the list.

   A new document is created with the settings (and objects) stored in the Style Sheet or Stationery Pad.

ChemDraw provides pre-defined Style Sheets or Stationery Pads located in the ChemDraw Items folder. For example, the ACS Document 1996 is configured to create documents that are set with the bond lengths, bond width, spacing, and fonts used in the 2-column format of all American Chemical Society journals. For a list of the settings stored in these documents, see Appendix G: "Document Settings".

NOTE: *Predefined Style Sheets or Stationery Pads may restrict your options in unexpected ways. For example, not all Save As... format options are available in all Style Sheets or Stationery Pads. For general use, you should stay with the default Style Sheet or Stationery Pad.*

Opening a Document

To open a document:

- From the **File** menu, do one of the following:
  - Choose **Open**, and in the Open dialog box, select the name and location of the file and then click **Open** or **OK**.
  - Choose the document from the list of previously opened documents at the bottom of the menu.

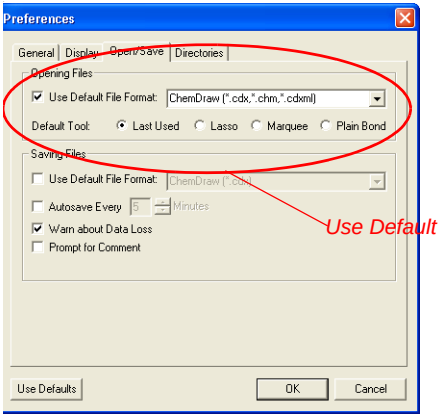
Setting the Default Open File Format

You can set what file format is selected by default in the Open dialog box.

To set the default file format:

1. From the **File** menu, choose **Preferences**.

   The Preferences dialog box appears.
2. Click **Open/Save**.
3. In the **Opening Files** section, click **Use Default File Format** and choose the format you want from the list



If **Use Default File Format** is not selected, the first time you use the Open dialog box the ChemDraw format is shown. Subsequent uses show the last format used.

Saving Changes Automatically

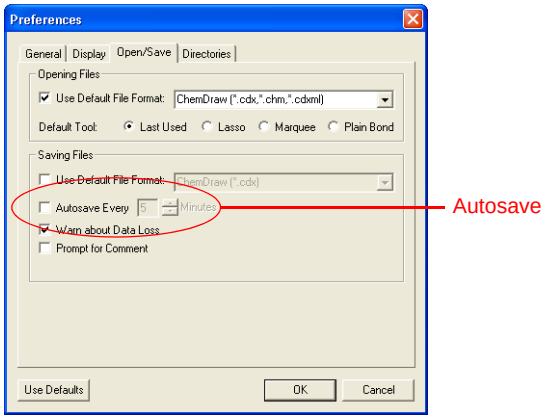
You can configure ChemDraw to save changes to a document automatically at the time interval you set.

To set the frequency at which ChemDraw automatically saves your changes:

1. From the **File** menu, choose **Preferences**.

   The Preferences dialog box appears.
2. Click **Open/Save**.

3. Click the checkbox next to **Autosave Every** and type or select the minutes to use.



The time starts counting down after the first change is made.

Reversing and Repeating Actions

ChemDraw keeps track of the actions you perform. You can reverse actions one at a time by choosing the Undo command. The number of actions that can be undone or redone is limited only by the amount of memory (RAM and virtual memory) available for use by ChemDraw. When you save your document the Undo queue is reset and starts over.

Undoing Actions

To undo the last action performed:

- From the **Edit** menu, choose **Undo**.

  The last action performed is reversed. The Redo command changes to reflect the undone action. The Undo command changes to reflect the next action you can undo.

For example, if you draw cyclohexane, create an atom label text box, type a label, and select and rotate the structure, you will be able to remove the actions as follows:

1. Remove the rotation.
2. Remove atom label.
3. Remove the ring.

At each step, the text of the Undo command indicates the action being removed.

Redoing Actions

When you undo an action, the Redo command becomes active so you can reverse the effect of the Undo command.

To redo the last action undone:

- From the **Edit** menu, choose **Redo**.

  The last action undone is reinstated. The Undo command changes to reflect that action. The Redo command changes to reflect the next action that can be redone.

Repeating Actions

If an action is repeatable, the name of the action appears next to the Repeat command on the **Edit** Menu.

To repeat an action:

- From the **Edit** menu, choose **Repeat**.

  The last action performed is repeated.

Discarding Recent Changes to a Document

To retrieve the last saved version of a file:

- From the **File** menu, choose **Revert**.

All changes made to the file since it was saved last are discarded and the previous version of the file appears.

NOTE: *You can use the Undo command in the Edit menu to remove each individual action since the last save.*

Saving Documents

To save a ChemDraw document in the default ChemDraw .cdx file format:

1. From the **File** menu, choose **Save**.

   The **Save** dialog box appears. The appearance of the dialog box depends on the platform you are using.
2. Choose a folder in which to store the file.
3. Type a file name in the File name (Windows) or Save As (Macintosh) text box. You may type up to 255 characters for a file name, including spaces. For example: "my first structure in ChemDraw".
4. Click **Save** or **OK** to create the file.

   The title of the document window changes to the name of the saved file. The file name is added to the bottom of the **File** menu.

CAUTION

ChemDraw uses the .cdx file format to store chemical information accurately with a structure drawing. Other file formats may be capable of storing a picture of your drawing, but they might lose chemically relevant information about the structure. For example, if you save a ChemDraw drawing in the .eps file format, you will store only a picture of the structure without storing the chemical significance of the connections between atoms and bonds.

To save a document that has previously been saved:

- From the **File** menu, choose **Save**.

  The contents of the file are updated to reflect the information currently in the window without displaying the Save As dialog box.

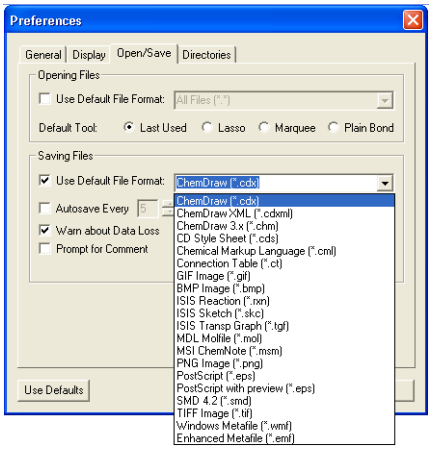
Setting the Default Save File Format

You can set what file format is selected by default in the Save As dialog box.

To set the default file format:

1. From the **File** menu, choose **Preferences**.

   The Preferences dialog box appears.
2. Click **Open/Save**.
3. In the **Saving Files** section, click the checkbox next to **Use Default File Format** and choose the format you want from the list.



If **Use Default File Format** is not selected, the first time you use the Save dialog box, the ChemDraw format is shown.

Saving a Document with a Different Name or Location

You can save a copy of your document under a different name, location, or file format. Saving a copy under a different name or location is useful for keeping earlier revisions of your document. Saving

a file as a different format is useful for creating Style Sheet or Stationery Pad and for exporting information to other applications.

To save a copy of a ChemDraw document under a different name or in a different location:

1. From the File menu, choose **Save As**.

   The Save As dialog box appears.
2. Choose a new location in which to save the document.
3. Type a new file name.
4. Click **Save** or **OK**.

Saving a Document in a Different File Format

To save a ChemDraw document in another file format:

1. From the File menu, choose **Save As**.

   The Save As dialog box appears.
2. Select a folder in which to save the document.
3. Type a file name in the in the File name or Save As box.
4. Select a file format from the File Format or Save as Format list.

NOTE: *When you select some formats, the Options button becomes active. Click it to open a dialog box for setting options specific to these formats. For more information about these options, see Chapter 12: "Sharing Information".*

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5. Click **Save** or **OK**.

If you type a name that already exists in the same directory, the existing document is replaced. If you do not want to replace the original ChemDraw document, use a different name. For information about other file formats, see Chapter 12: "Sharing Information".

Closing a Document

To close a ChemDraw document:

- From the File menu, choose **Close**.

If the document contains unsaved information, you are prompted to save the file.

Accessing Documents Quickly

You can access ChemDraw documents quickly by placing them in the ChemDraw Items folder and then selecting them from the Open Special menu.

You can access open documents quickly by using the Window menu.

The ChemDraw Items Folder

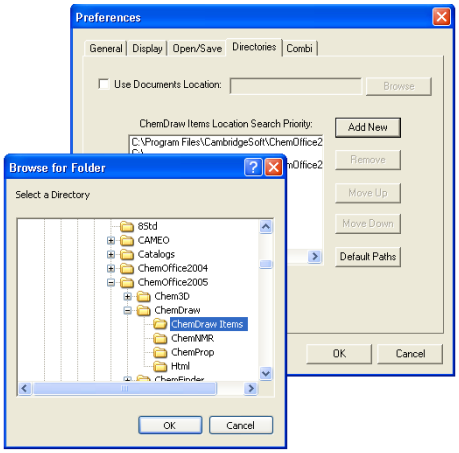
The ChemDraw Items Folder is located by default in the same folder as your ChemDraw application. It contains the ChemDraw preferences, hotkeys, nicknames, and isotopes files; scripts, and the generic nicknames file. It also contains template documents and template Stationery Pads. You can have multiple ChemDraw Items folders. This is useful in corporate installations for maintaining personal files such as nicknames as well as standard templates.

To add a path to a ChemDraw Items folder:

1. From the File menu, choose **Preferences**.

   The Preferences dialog box appears.
2. Click the **Directories** tab.
3. Click the **Add New** button, browse to a location, and click **OK**.

A new path is added to the list.



4. To rearrange the search order, use the **Move Up** and **Move Down** buttons.
5. To delete a path, click the **Remove** button. To delete all added paths, click the **Default Paths** button.

The Open Special Submenu

To select documents from the ChemDraw Items folder:

- On the **File** menu, point to **Open Special**, and select the file to open.

  The **Open Special** submenu, listing documents stored in the ChemDraw Items folder, appears.

The Window Menu

The **Window** menu lists all open ChemDraw and Template documents. The document you choose from the **Window** menu becomes the active window.

Printing

ChemDraw uses the standard system commands to print ChemDraw documents. The options that you have available to you depend on the printer that you are using. Refer to your printer's documentation for more information.

In general, to print a ChemDraw document:

1. From the **File** menu, choose **Page Setup**.
2. Make all appropriate selections for the printer you are using and click **OK**.
3. From the **File** menu, choose **Print**.
4. Make your selections in the Print dialog box and click **OK**.

To print a document from the Explorer or from the Finder:

1. Select the document you want to print.
2. From the **File** menu, choose **Print**.

   The ChemDraw application is opened and the Print dialog box appears.
3. Make your selections in the Print dialog box and click **OK**.

Printing Background Color

Print Background Color controls whether the Background Color contained in your ChemDraw document is printed.

To change whether the Background color is printed:

1. From the **File** menu, choose **Preferences**.
2. Click **Print Background Color**.
3. Click **OK**.

Macintosh Print Preferences

When you print a document, ChemDraw creates both a QuickDraw representation and a PostScript representation of the document's contents.

QuickDraw is the graphical format that is supported by the Macintosh Operating System. Every printer that supports the MacOS can convert QuickDraw representations into printed output. However, QuickDraw does not support some features (for example, high-resolution printing) that are available only on some printers.

If you are transferring information to another application from which you print ChemDraw pictures, you should consider including PostScript commands and the ChemDraw LaserPrep File with the pictures. For information about special situations to consider, see "Transferring PostScript (Macintosh)" on page 195.

Optimize Pictures for High-Resolution Non-PostScript Printing

The Macintosh High Resolution Clipboard supports high-resolution printers. Most applications support the High Resolution Clipboard. Because this was not always the case in the past, this preference continues to be available for users to turn off if an application being used does not support the High Resolution Clipboard.

If you are unsure if the application uses a High Resolution Clipboard, try transferring pictures with this check box selected and deselected, and see which picture prints with higher quality.

If you are printing to a non-PostScript printer, deselect **Include ChemDraw LaserPrep** and **Include PostScript** to reduce the size of each picture. Do not deselect this option if the document will ever be printed to a PostScript printer.

Printers that use the PostScript page definition language use the PostScript representation. The PostScript representation describes objects by using mathematical shapes that can be precisely imaged at whatever resolution is used by your printer. The PostScript representation created by ChemDraw is composed of two parts, the PostScript commands and the ChemDraw Laser Prep. The ChemDraw Laser Prep contains specific instructions that enable the printer to interpret the PostScript commands contained in a ChemDraw document.

Include PostScript

To transfer ChemDraw pictures to another document that will be printed on a PostScript printer:

1. From the **File** menu, choose **Preferences**.
2. Click **Include PostScript**.
3. Click **OK**.

When Include PostScript is deselected, no PostScript commands are generated. This usually results in lower quality printing, particularly of drawings cut and pasted into other applications. However, because the representation used for printing when Include PostScript is not selected is the same as that used for drawing to the screen, better correspondence between the screen and printed output may be observed.

For more information, see "Transferring PostScript (Macintosh)" on page 195.

Include ChemDraw Laser Prep

Selecting the include ChemDraw Laser Prep allows you to print to a printer that cannot be initialized using ChemDraw. If you create drawings with this option off, they will not print on PostScript printers without the use of ChemDraw.

To Include ChemDraw Laser Prep:

1. From the **File** menu, choose **Preferences**.
2. Click **Include ChemDraw Laser Prep**.
3. Click **OK**.

NOTE: *When you select Include ChemDraw Laser Prep, you should also select Include PostScript.*

For more information, see "Transferring PostScript (Macintosh)" on page 195.

Scripts (Macintosh)

The **Scripts** menu contains scripts that you can use to perform tasks within ChemDraw or between ChemDraw and another scriptable application.

Scripts, found in the **Scripts** menu, are created using Apple's Script Editor application. With the proper script extensions in conjunction with Apple's Script Editor application, you can create scripts using the AppleScript™ scripting language and add scripts to the **Scripts** menu by placing them in the ChemDraw Folder.

NOTE: *Scripts not stored within the ChemDraw Folder are not accessible from the Scripts menu.*

For more information about AppleScript™ and the Script Editor application see your system manuals.

Closing ChemDraw

To close the ChemDraw application:

- From the **File** menu, choose **Exit ChemDraw** or **Quit ChemDraw**.

  If you have unsaved document windows open, you are prompted to save them before you can close the application.

Chapter 2: Tutorials

Overview

The tutorials are designed to teach you the fundamental drawing techniques available in ChemDraw. Before you begin, you may want to review "Conventions" on page 10 to familiarize yourself with the terminology used in the tutorials. You may also want to use your Quick Reference Card while you perform the tutorials.

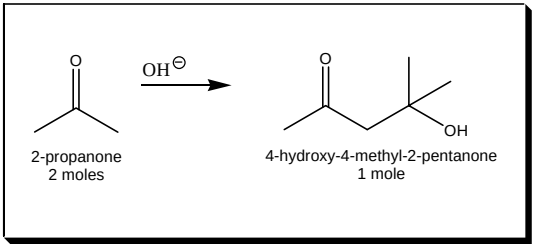
ChemDraw automatically checks for correct chemical syntax as you draw. If ChemDraw finds a potential problem, a red box is displayed around the erroneous object. The red box is displayed on screen only and does not print.

To disable the automatic warning on a specific object:

- Right-click the object and deselect **Display Warnings**.

Tutorial 1: Reaction Schemes

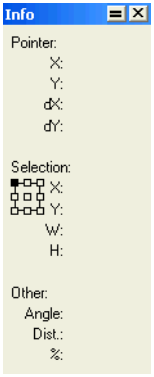
In this tutorial, you will draw the following (simplified) reaction scheme:



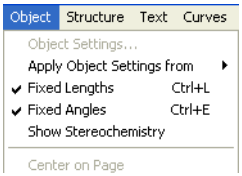
Create a ChemDraw Document:

1. Start ChemDraw.
2. From the **File** menu, choose **Save As**.
3. Type tut1.cdx in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.
6. From the **View** menu, choose **Show General Toolbar**.
7. From the **View** menu, choose **Show Info Window**.

   The Info window appears and displays drawing parameters as you draw.



8. Click the **Object** menu and make sure there is a check mark next to the **Fixed Lengths** and **Fixed Angles** commands. If either command is not checked, select it.

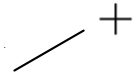


NOTE: *Applying fixed lengths and fixed angles enables you to create structures with consistent bond lengths and angles. The fixed length dimension is set in the Drawing Settings dialog box. The fixed angle dimension increments angles by 15 degrees.*

Create a bond:

1. Click the Solid Bond tool .
2. Position the pointer (+) anywhere in the document window and click.

   The bond is extended to its fixed length at a 30-degree angle.



Add a second bond:

1. Point to the right atom of the bond.

2. Click the atom to add a bond.

   A second bond is drawn, forming a 120-degree angle between the bonds.

NOTE: *The angle used when clicking to add bonds is controlled by the Chain Angle setting in the Drawing Settings dialog box in the File menu. If this bond angle cannot be established, the next smaller and logical bond angle is used.*

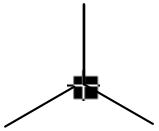
Add a third bond:

1. Continue pointing to the atom shown below.

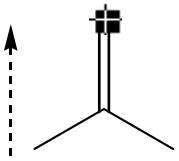
2. Click the atom to add a bond.

Change a single bond into a double bond:

1. Point to the atom shown below and hold the mouse button down.

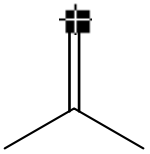


2. Drag as shown below over the existing single bond. Release the mouse button.

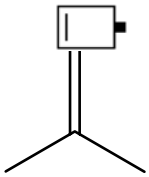


Add labels to the structure:

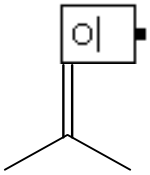
1. Point to the atom shown below.



2. Double-click the atom.



3. Type an uppercase O in the text box that appears.



4. Close the text box by doing one of the following:
   - Click in an empty area of the window.
   - Click another tool.

Next, you duplicate a structure and then create another structure from the duplicate.

Duplicate the structure:

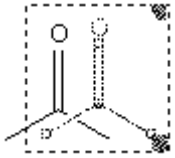
1. Click the Lasso tool .

   The last structure drawn is automatically selected.
2. Point over the Selection Rectangle.

3. Press and hold **Ctrl** or **Option**.

   The hand pointer with a plus sign indicates that you are in the duplication mode of a selection tool.

4. Drag the Selection Rectangle to the right.

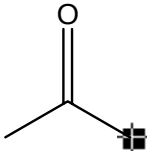


   A copy of the structure appears as you begin drag. The original structure remains in its position. Release the mouse button when the copy is clear of the original.

NOTE: *When you create a copy as shown above you can drag it anywhere in the document window. If you want the copy to remain aligned with the original, hold Shift while dragging.*

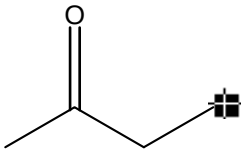
Modify the duplicated structure:

1. Click the Solid Bond tool .
2. Point, in the copied structure, to the atom shown below and click.



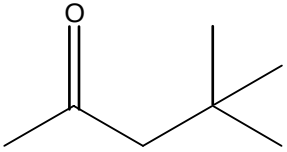
Add several bonds to a single atom:

1. Point to the atom shown below.



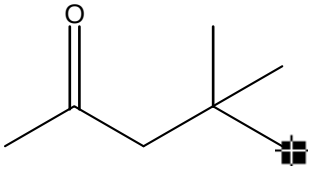
2. Click the atom three times, allowing a pause between each click.

> ***NOTE:*** *If you click too fast, the click is interpreted either as a double-click, which opens a text box or a triple-click, which duplicates your last atom label.*

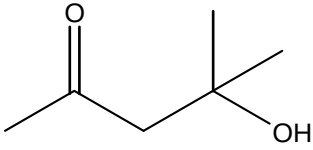


Create an atom label using HotKeys. HotKeys are keys on your keyboard that are linked to specific atom labels. For more information about HotKeys, see "Labeling Atoms with HotKeys" on page 87.

1. Point to the atom shown below.



2. Type O or o.

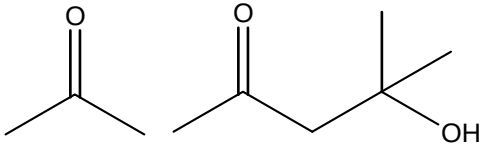


When you use HotKeys that represent a single element, the correct number of hydrogen atoms is added to the label.

Align the structures:

1. Select the structures.
2. On the **Object** menu, point to **Align**, and then choose **T/B centers**.

You structures should appear as shown below.



In the following steps, you use a different method for selecting structures and then separate the structures to make room for an arrow.

1. Click the Marquee tool .

> ***NOTE:*** *Alternatively, you can select the Lasso tool and hold Alt or Option to use the Marquee tool.*

The last object drawn is selected.

Drag the selection to make room for an arrow:

- Press **Shift** to maintain the alignment of the structure and drag the Selection Rectangle to the right.

Add arrows to the reaction scheme.

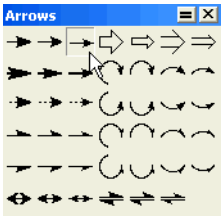
1. Click the Arrow tool to display the Arrow palette.

> ***NOTE:*** *The triangle in the lower right corner of the Arrow icon indicates it contains a palette.*

2. Holding the mouse button down, move the mouse to the palette title bar, then release the mouse button.

   The palette becomes a floating tool bar. Drag the palette to the location you want.

3. Click the third arrow from the left in the top row.

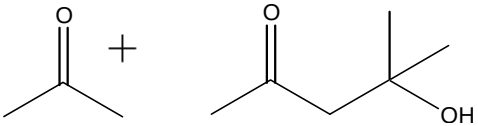


4. After the arrow is selected, release the mouse button.

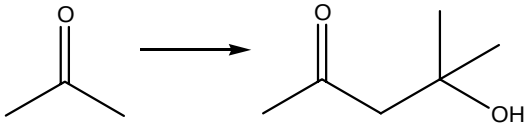
NOTE: *The arrow you choose from the palette becomes the default arrow type. To change the arrow type, display the arrow palette and select the arrow type you want.*

Draw the arrow you selected:

1. Point after the first structure and hold down the mouse button.



2. Drag the Arrow to the length you want. Release the mouse button.

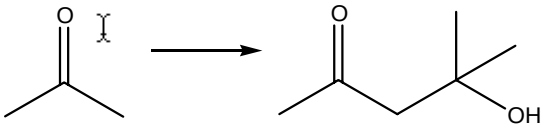


NOTE: *If you need to change the length (or the angle relative to the X-axis) of the arrow:*
1. Hold Shift and point to the arrowhead (a highlight box appears when you are pointing correctly).
2. Drag the arrowhead to the length (and angle) you want.

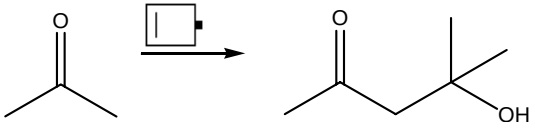
Use the Text tool to add line formula or other captions for representing reagents and reactions.

Insert text in the drawing:

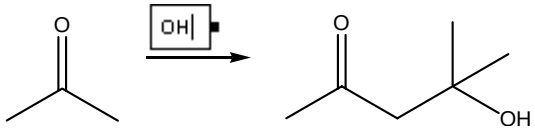
1. Click the Text tool A.
2. Point above the arrow. A text insertion point appears as shown below.



3. Click to create a text box.



4. Type OH.



NOTE: *If you want to realign the caption, select a selection tool and drag the caption.*

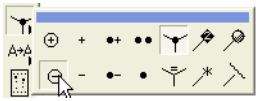
Add a charge symbol using the specialized symbols available in the Chemical Symbols tool palette:

1. Click the Chemical Symbol tool.

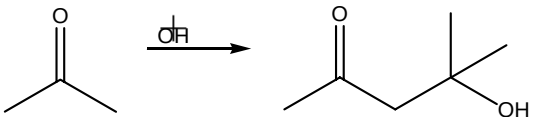
NOTE: *A red box appears around the OH label indicating an error, i.e. that you haven't added the charge yet.*

---

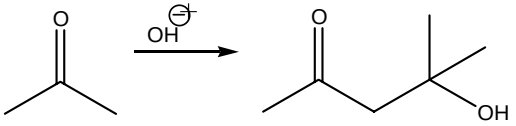
2. Holding the mouse button down, select the circled **negative charge symbol** shown below, then release the mouse button.



3. Point to the center of the OH label. Moving the cursor slightly right or left will cause either the O or the H to be selected.



4. With the H selected, drag the charge symbol around the atom to the desired position.

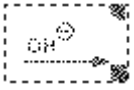


Objects added from the Chemical Symbols palette are automatically associated with the structure they are closest to.

Some objects, such as arrows, are not associated automatically. You can manually group objects using the Group command. You can then select the grouped objects to manipulate or move them together.

To group objects:

1. Click a Selection tool, the Lasso or Marquee tool.
2. Hold Shift and click the arrow, the OH caption, and the charge symbol.



The Shift key allows you to add objects to a selection without deselecting other objects.

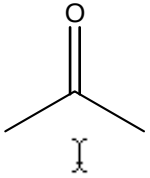
NOTE: *If you click a selected object while holding Shift, that object is deselected.*

3. From the **Object** menu, choose **Group**.

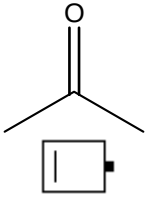
NOTE: *You can select individual objects within a group by clicking them.*

Use the Text tool to create a caption containing the name and amount of reactant, and then center the caption under the structure.

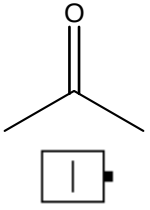
1. Click the Text tool A.
2. Point below the first structure.



3. Click to create a text box. The default cursor is flush left.



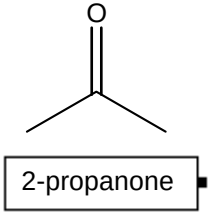
4. From the **Text** menu, choose **Centered**.



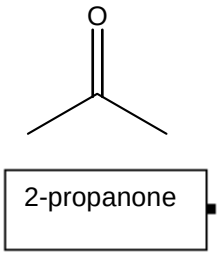
The cursor moves to the center of the text box.

Type the caption:

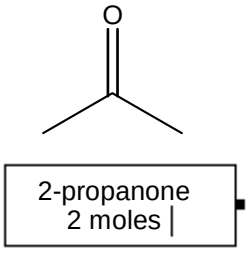
1. Type 2-propanone.



2. Press the **Enter** or **Return** key to insert a new line.

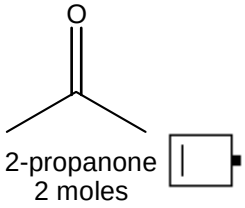


3. Type 2 moles.



Create an aligned caption for the other structure.

1. Press the **Tab** key to create another Text box that is aligned adjacent to the first.



NOTE: *You can use the Tab key in the caption mode of the text tool to create multiple aligned captions with the same font, font size, style, and justification as the previous caption.*

2. Type 4-hydroxy-4-methyl-2-pentanone, press the **Enter or Return** key, and then type 1 mole.

If your captions are not aligned properly beneath the structures you can move them using a selection tool.

1. Click a Selection tool (Lasso or Marquee).

   The text box is automatically selected because it is the last object drawn.

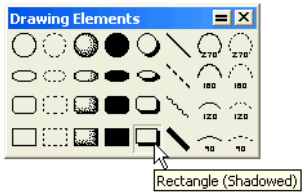
NOTE: *The object that is automatically selected is set in the Preferences dialog box.*

2. Press the **Left** or **Right Arrow** key to center the caption beneath its structure. This method maintains the alignment created by the Tab key.

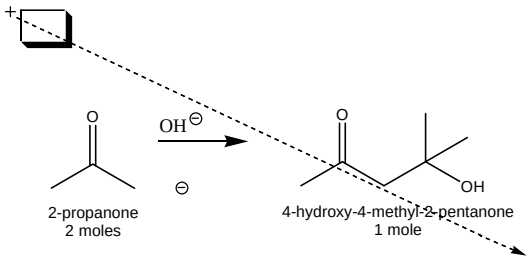
To complete the drawing, add a shadowed box around the scheme:

1. Click the Drawing Elements tool .

2. Select the **shadowed box** from the palette of drawing elements.



3. Point to the upper left corner of the reaction scheme. Hold the down the mouse button and drag diagonally downward to the right to draw the box.

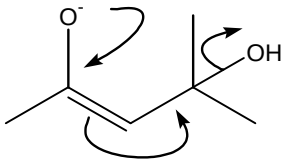


Save and close the document:

1. From the **File** menu, choose **Save**.
   Your document is saved.
2. From the **File** menu, choose **Close**.

Tutorial 2: Drawing an Intermediate

In this tutorial you will draw the following intermediate structure starting from a ring and then add arrows with customized shapes using the Pen tool.

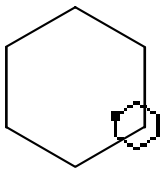


Create a new ChemDraw document:

1. From the **File** menu, choose **New Document**.
2. From the **File** menu, choose **Save As**.
3. Type tut2.cdx in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.

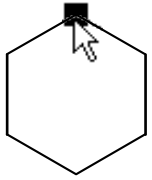
Draw a ring:

1. Click the Cyclohexane Ring tool .
2. Point in the document window. The Cyclohexane cursor appears.
3. Click to add a ring.

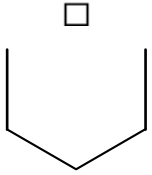


Delete an atom and its bonds from the ring:

1. Click the Eraser tool .
2. Point to the atom shown below.



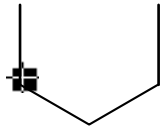
3. Click the atom.



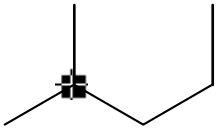
NOTE: *You can delete a bond individually by pointing at the center of the bond and clicking.*
You can also drag the eraser to make multiple deletions.

Add a bond:

1. Click the Solid Bond tool .
2. Point to the atom shown below.

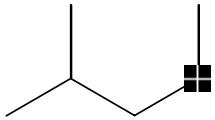


3. Click to add a bond.

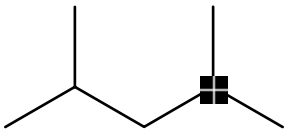


Add second and third bonds:

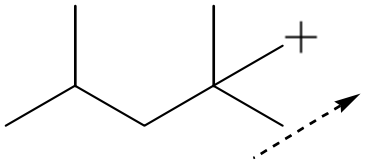
1. Point to the atom shown below and click to add another bond.



2. Add a third bond by dragging to make sure it has the desired orientation:
   a. Continue pointing to C4.



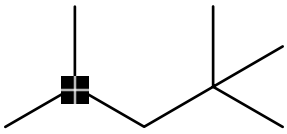
   b. Hold the mouse button and drag diagonally upward toward the right.



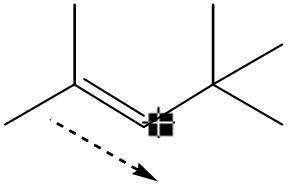
   c. When the bond is oriented, release the mouse button to deposit the bond.

Create a double bond:

1. Point to the atom shown below.

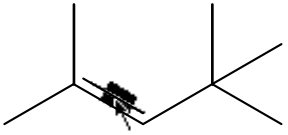


2. Drag diagonally downward over the existing bond to create a double bond.



Change the orientation of the double bond:

1. Point to the center of the double bond.



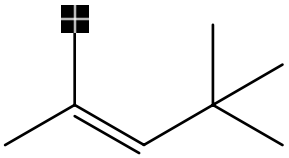
2. Click the bond twice to move the second line to the outside.

   The bond moves to the inside on the first click and to the outside on the second click

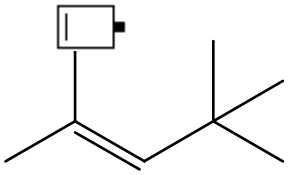
NOTE: *You can move a double bond by clicking it when a bond tool is selected. The cursor corresponding to the bond tool that is selected appears.*

Add an atom label:

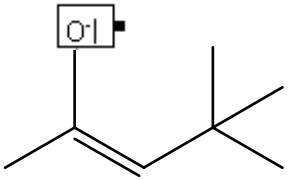
1. Point to the atom to label shown below.



2. Double-click the atom to open a text box.

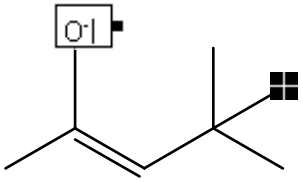


3. Type O and then type "-".

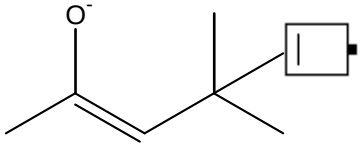


Label an atom with OH:

1. Point to the atom shown below.



2. Double-click the atom to open a text box.



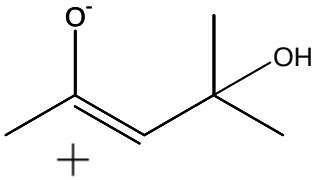
3. Type OH.

Next you will add an arrow that is not included in the arrow palette to indicate electron flow.

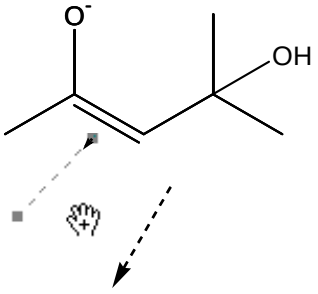
To create a customized arrow using the Pen tool.

1. Click the Pen tool .
2. From the **Curves** menu, choose **Arrow at End**.

3. Point near the double bond where you want to indicate the start of electron flow.

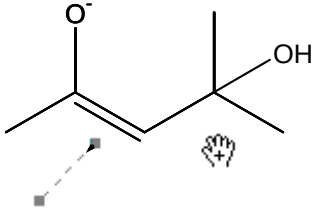


4. Drag downward and to the left. Release the mouse button.

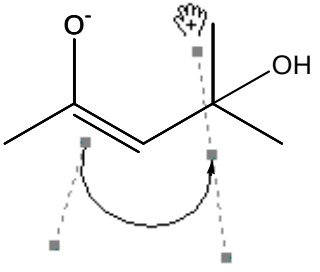


The hand with a "+" cursor indicates that you are in the editing mode of the Pen tool.

5. Position the cursor where you want the arrowhead to appear.

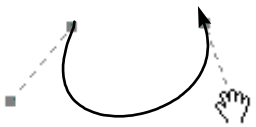


6. Drag upward to create a curve segment.

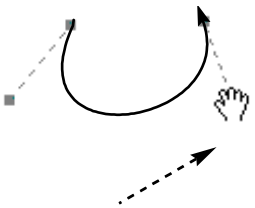


Refine the shape of the arrow:

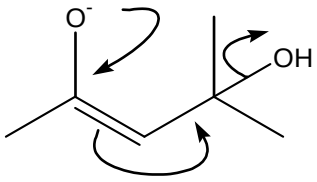
1. Point to the handle pointing away from and to the right of the curve. This is a tangent handle that controls the tangent of the curve that it touches.



2. Drag the handle upward to the right to make the arrowhead point more inward.



3. Press **Esc** when you are finished.
4. Create additional arrows as described above to complete the intermediate as shown below.



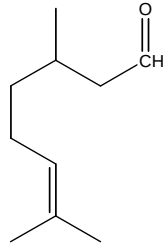
NOTE: *If you want to magnify the entire document so you can see arrows or other objects that are in small places, choose Magnify from the View menu.*

Save and close the document:

1. From the **File** menu, choose **Save**.
2. From the **File** menu, choose **Close**.

Tutorial 3: Using Rings

In this tutorial you will draw more complex structures by using rings.



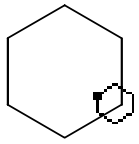
Open a new ChemDraw document:

1. From the **File** menu, choose **New Document**.
2. From the **File** menu, choose **Save As**.
3. Type tut3.cdx in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.

Create a ring:

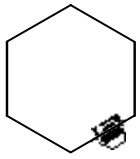
1. Click the Cyclohexane Ring tool .
2. Point in an empty area of a document window.

3. Click to add a ring.

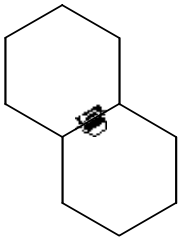


Fuse a second ring to the first:

1. Point to the center of lower right bond in the ring.

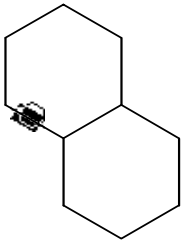


2. Click to fuse another ring.

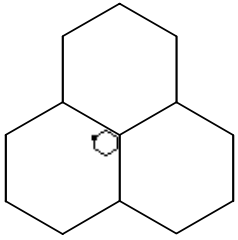


Fuse a third ring:

1. Point to the bond shown below.

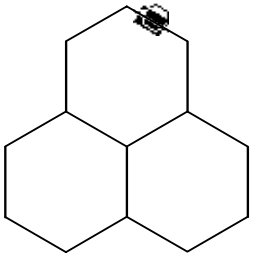


2. Click to fuse another ring. Your document should contain the structure shown below.

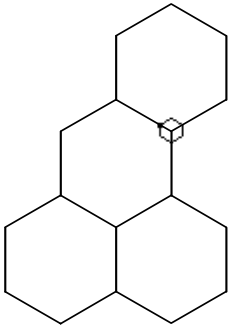


Fuse a fourth ring:

1. Point to the bond shown below.

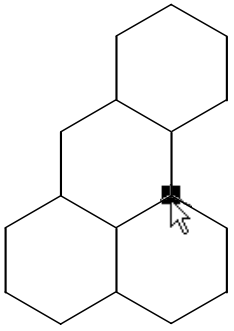


2. Click to fuse another ring.

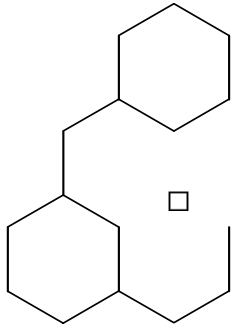


Remove atoms and their bonds from the ring using the Eraser tool:

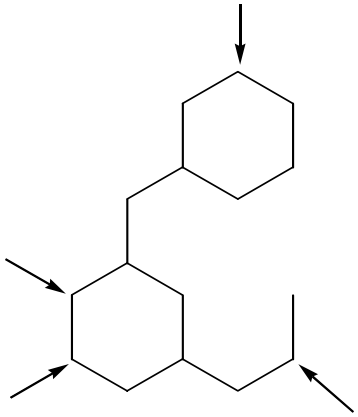
1. Click the Eraser tool .
2. Point to the atom shown below.



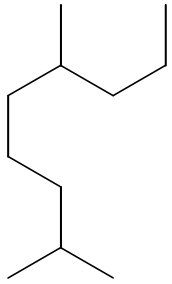
   A highlight box appears on the atom to be removed.
3. Click to delete the atom and its bonds.



4. Click each of the atoms shown below to delete the bonds.

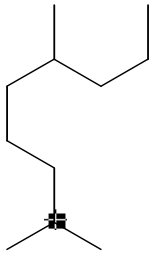


The resulting structure is shown below.

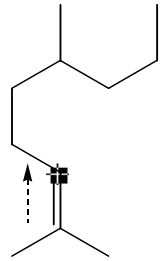


Add double bonds to the structure:

1. Click the Solid Bond tool .
2. Point to the atom indicated below.

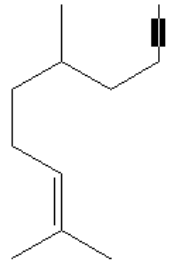


3. Drag upward to draw a double bond.



Add another double bond:

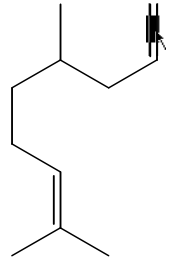
1. Point to the bond shown below.



2. Right-click, point to **Double,** and then choose **Plain**.

Realign the double bond so it is centered:

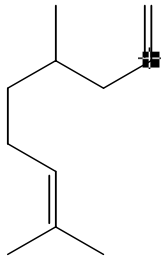
1. Point to the center of the upper double bond.



2. Right-click, point to **Bond** position, and then choose **Centered**.

Add a carbon atom label:

1. Point to the atom shown below.

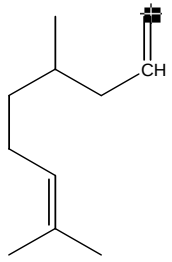


2. Press the **c** key on your keyboard. "c" is a Hotkey assigned to the atom label C.

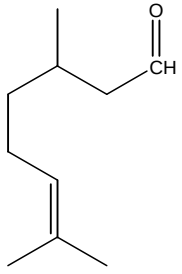
   The CH atom label appears with the correct number of hydrogen atoms.

Add an oxygen atom label to complete the structure:

1. Point to the atom shown below.



2. Press the **o** key on your keyboard. "o" is a Hotkey assigned to the atom label O.

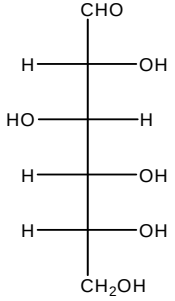


Save and close the document.

1. From the File menu, choose **Save**.
2. From the File menu, choose **Close**.

Tutorial 4: Fischer Projections

This tutorial demonstrates creating a Fischer projection of glucose (shown below) by drawing a linear series of bonds. You can also create the same drawing using a template.



Create a document from a template by opening the appropriate document template:

1. From File menu, point to Open Special, and then choose **ACS Document 1996**.

   The new document created is based on a Style Sheet or Stationery Pad.

NOTE: *These special documents allow you to have pre-configured settings for different tasks. In this example, the ACS template provides the required settings for structures to be published in all ACS journals:*

- *One-column layout (Page Setting)*
- *Bonds with a Fixed length of 0.2 inches (Drawing Setting)*
- *Atom Labels in 10 point Arial or Helvetica font (Text Setting)*

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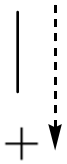
2. From the File menu, choose **Save As**.
3. Type tut4.cdx in the appropriate text box.

4. Select a folder in which to save the file.
5. Click **Save**.

Draw the first bond:

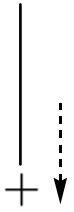
1. Click the Solid Bond tool .
2. Point in the document window. Drag downward vertically to draw the first bond.



Add a second bond:

1. Point to the lower atom.

2. Drag downward to draw the second bond.



3. Repeat step 1and step 2 three times to draw a total of five bonds.

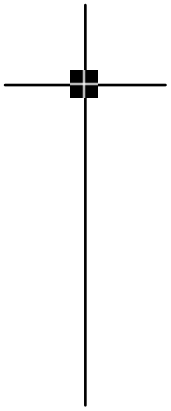
NOTE: *When you drag the pointer along the length of the bonds, the pointer alternates between an arrow and a cross. The arrow indicates you are pointing over the center of a bond, and the cross indicates you are pointing to an atom.*

Add horizontal bonds to the second atom in the string of bonds you created:

- Point to C2 and click the atom to add a perpendicular bond.

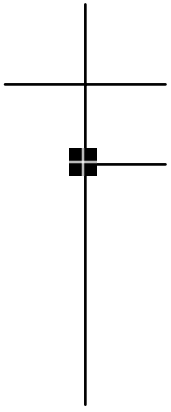
Add a horizontal bond in the opposite direction:

- Continue pointing to C2 and click the atom to add a perpendicular bond in the opposite direction.

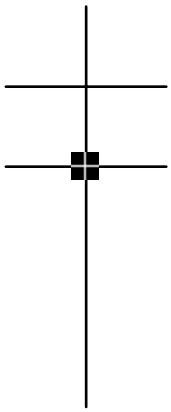


Add bonds to the next three carbon atoms:

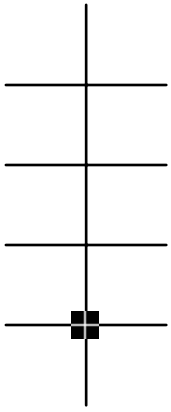
1. Point to C3 and click the atom to add a perpendicular bond.



2. Continue pointing to C3 and click the atom to add a perpendicular bond in the opposite direction.

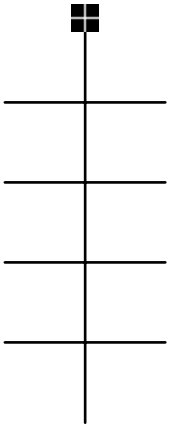


3. Repeat step 1 and step 2 for the fourth (C4) and fifth (C5) atoms.

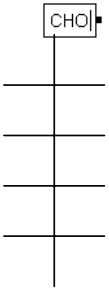


Add labels to C1 and C6:

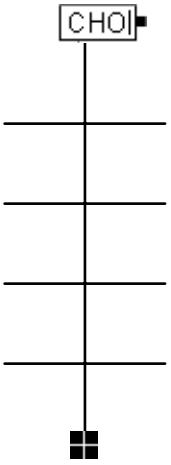
1. Point to C1.



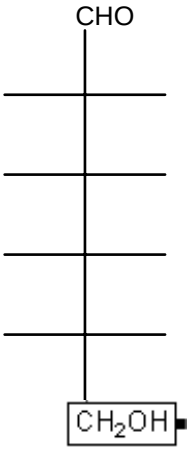
2. Double-click C1 to create a text box, then type CHO.



3. Point to C6.

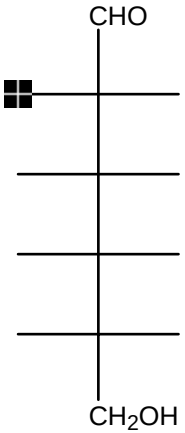


4. Double-click C6 to create a text box, then type CH2OH.

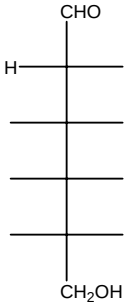


5. Type **Esc** to deselect the label.
6. Add the H and OH labels:

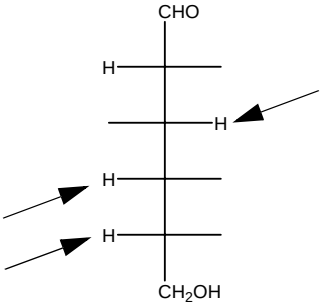
1. Point to the atom shown below.



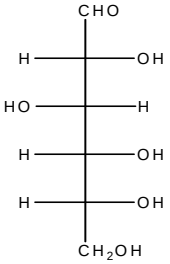
2. Type h to label the atom using the Hotkey label for hydrogen.



3. Repeat step 2 for the remaining hydrogen atoms shown below.



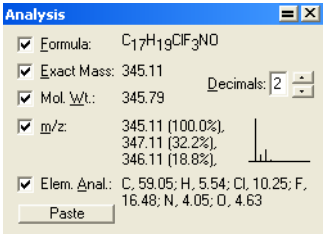
4. Label the remaining atoms by typing o to label them with OH. The result should appear as shown below.



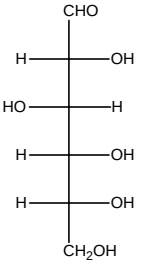
View the basic properties of the structure you drew and paste the information into your document:

1. Click a selection tool to automatically select the last structure drawn. If the structure is not selected, double-click the structure.
2. From the View menu, choose **Analysis Window**.

   The Analysis window appears. You can drag the window to any position.


Analysis
Formula: C17H19ClF3NO
Exact Mass: 345.11
Mol. Wt.: 345.79
Decimals: 2
m/z: 345.11 (100.0%), 347.11 (32.2%), 346.11 (18.8%),
Elem. Anal.: C, 59.05; H, 5.54; Cl, 10.25; F, 16.48; N, 4.05; O, 4.63
Paste

3. Click **Paste** to paste the information as a caption below the structure.



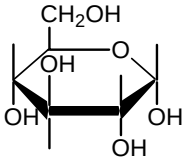
$C_6H_{12}O_6$
Exact Mass: 180.06
Mol. Wt.: 180.16
m/e: 180.06 (100.0%), 181.07 (7.1%), 182.07 (1.4%)
C, 40.00; H, 6.71; O, 53.29

Save and close the document:

1. From the **File** menu, choose **Save**.
2. From the **File** menu, choose **Close**.

Tutorial 5: Perspective Drawings

In this tutorial you will learn how to create a perspective drawing by drawing the following α-D-glucose as a Haworth projection.



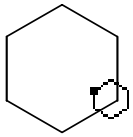
Create a new document using the ChemDraw default style:

1. From **File** menu, point to **Open Special**, and then choose **New Document**.
2. From the **File** menu, choose **Save As**.
3. Type tut5.cdx in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.

Draw a ring:

1. Click the Cyclohexane Ring tool .
2. Point in an empty area of a document window.

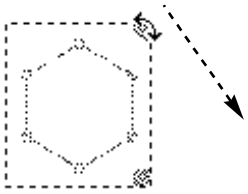
3. Click to add a ring.



Rotate the ring:

1. From the **Edit** menu, choose **Select All**.

2. Point to the upper right corner of the Selection Rectangle (the Rotation handle).



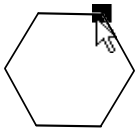
NOTE: *The cursor changes to a curved double-sided arrow to indicate the rotation mode of a selection tool is activated.*

3. Drag the Rotation handle to the right about 30 degrees. The amount of rotation is displayed on the screen and in the Info window.

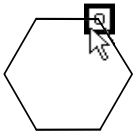
Even though Fixed Angles is on, the angle is not constrained. The Fixed Angles feature constrains angles only when they are being drawn. For example, if you created this ring by dragging instead of clicking, the angle would be constrained when Fixed Angles is on.

Change cyclohexane to tetrahydropyran:

1. Click outside the structure to deselect it.
2. Point to the atom indicated below.

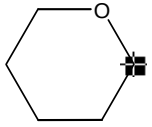


3. Type o.

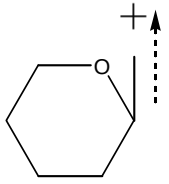


Add vertical bonds:

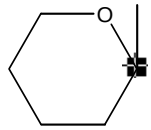
1. Click the Solid Bond tool .
2. Point to the atom shown below.



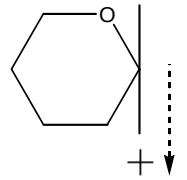
3. Drag upward to create a bond.



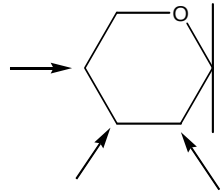
4. Point to C1 again.



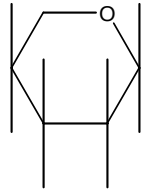
5. Drag downward to create another bond.



6. Repeat for the atoms indicated by the arrows below.

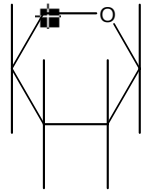


The result appears as shown below.

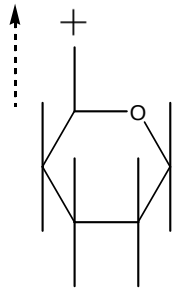


Draw one bond upward at C5:

1. Point to the atom shown below.



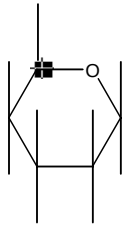
2. Hold the mouse button and drag upward.



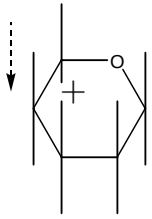
For the downward bond for C5, you must turn Fixed Lengths off or the bond will be joined to the upward bond of C3.

You can temporarily disable **Fixed Lengths** using a modifier key:

1. Point to the atom shown below.

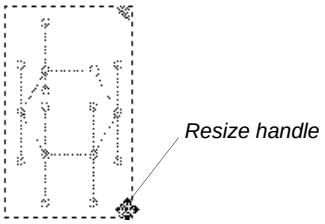


2. Hold down the mouse button, press the **Alt** or **Option** key and drag downward from C5. Stop dragging about half the distance to the upward bond on C3.



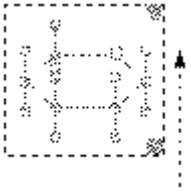
Distort the structure to change its aspect ratio to give the perspective of viewing the structure along the Z-axis.

1. Click the Lasso tool .
2. Point to the Resize handle (lower right corner) and press the **Shift** key.



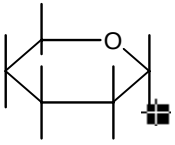
NOTE: *The cursor changes to a cross with arrows at each end indicating the distortion function of a selection tool.*

3. Drag upwards until you have distorted the structure to about 50%, as shown on the screen or in the Info window.

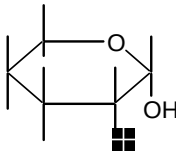


Next, you create OH labels. Because this label is repeatedly used, you will learn how to repeat a label. Only labels created by opening a text box are repeatable.

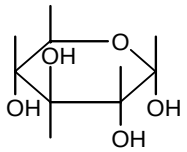
1. Select the Solid Bond tool, point to the atom shown below and double-click to open a text box.



2. Type OH, move the pointer to the next atom as shown, and triple-click to repeat the atom label.



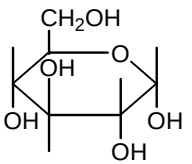
3. Triple-click the remaining atoms (as shown below) to repeat the OH label.



NOTE: *If you find it difficult to place the labels because of the size of the drawing, choose Magnify from the View menu.*

Add the CH_2OH label:

1. Triple-click the upper atom of C5.
2. Press the **Enter** or **Return** key to open the atom label text box and type CH2 before the OH.

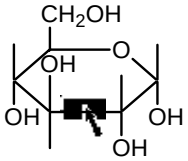


NOTE: *The Enter or Return Hotkey opens a text box for the last atom labeled. The definition for this particular Hotkey cannot be changed.*

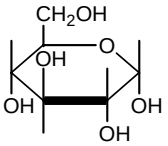
Change the type of the front bonds:

1. Click the Bold Bond tool .
2. Point to the center of the bond shown below.

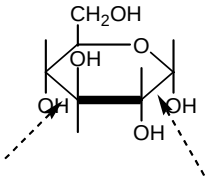
The cursor changes to a bold arrow as you point at the bond.



3. Click to change to the new bond type.



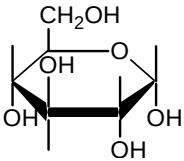
4. Click the Bold Wedge bond tool .
5. Point to each of the bonds shown below.



6. For each bond, point slightly off center in the direction that you want the wide end of the wedge to be oriented and click.

NOTE: *If you move the pointer too far, the highlight box disappears. Choose Magnify from the View menu if you find it difficult to place the pointer.*

The resulting structure is shown below.



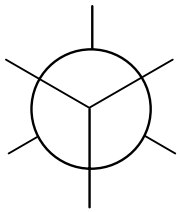
NOTE: *If the wedge is pointed in the wrong direction, click the bond again to flip its orientation.*

Save and close the document:

1. From the **File** menu, choose **Save**.
2. From the **File** menu, choose **Close**.

Tutorial 6: Newman Projections

This tutorial demonstrates how to draw a Newman projection. You can also create the same drawing using a template.



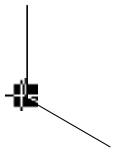
Create a ChemDraw document:

1. From the **File** menu, choose **New Document**.
2. From the **File** menu, choose **Save As**.
3. Type tut6.cdx in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.

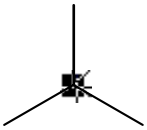
Create the first bond:

1. Click the Solid Bond tool .
2. Point in the document window and drag downward to create the first bond.

3. Continue pointing at the lower atom and click again to add a second bond.



4. Continue pointing at the same atom and click again to add a third bond.

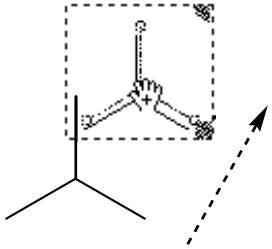


5. Click the Lasso tool .

   The last structure you drew is automatically selected.

6. Point within the Selection rectangle and hold the **Ctrl** or **Option** key.

7. Hold the mouse button and drag a copy of the structure diagonally upward to the right of the original.

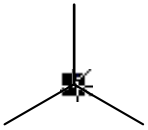


8. Release the mouse button and depressed key when the copy is positioned.

Add a bond between the duplicated structures:

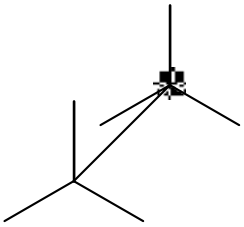
1. Click the Solid Bond tool .

2. Point to the central atom of the lower fragment.



NOTE: *When connecting existing atoms, the Fixed Length and Fixed Angles commands are ignored.*

3. Click and drag to the central atom of the upper fragment.
4. Release the mouse button when the highlight box over the central atom appears.

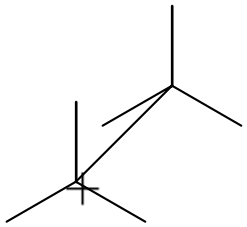


In this step, you will use the Orbital tool to draw the hollow circle that is particular to Newman Projections rather than an orbital.

1. Click the Orbital tool .
2. Click the unfilled s orbital.

3. Point to the left center carbon and drag outward.

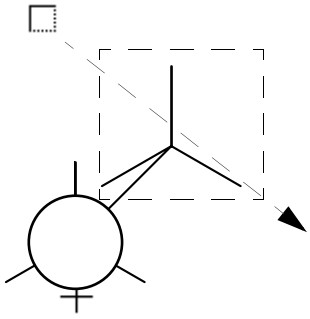
The size of the orbital is constrained just like bonds. The constraint is based on a percentage of the Fixed Length setting in the Drawing Settings dialog box.



NOTE: *Orbitals are not automatically grouped with the closest structure. If you want to group the orbital with the existing structure so you can move them as a unit, choose Group from the Object menu.*

Move part of the structure to the front to overlap the orbital:

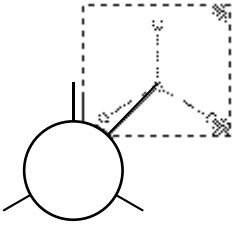
1. Click the Marquee tool .
2. Point above the structure and drag around the upper fragment to select the three bonds.



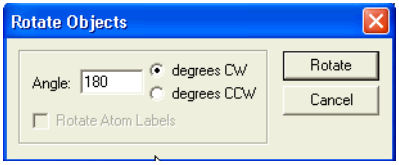
NOTE: *Only bonds that are completely within the Lasso area are selected. Do not select the bond connecting the two fragments. Alternately, you can Shift+click on each bond separately.*

Rotate the selection:

1. Double-click the Rotation handle in the upper right of the Selection Rectangle to open the Rotate dialog box.



2. Type 180 in the text box, select **degrees CW**, and then click **Rotate**.

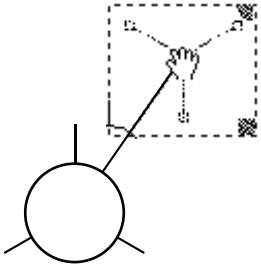


Change the layering of the structure so that the selection is in front:

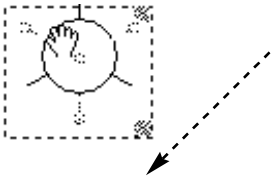
- From the **Object** menu, choose **Bring to Front**.

Orient the front part of the structure to create a Newman projection.

1. Point within the Selection Rectangle until the pointer changes to a hand.



2. Drag the selection until the central atom of the selection is centered within the orbital.



3. Release the mouse button and click outside the Selection Rectangle to deselect the structure.

Save and close the document:

1. From the **File** menu, choose **Save**.
2. From the **File** menu, choose **Close**.

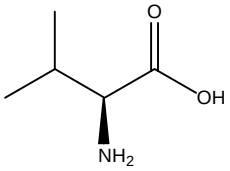
Tutorial 7: Showing Stereochemistry

This tutorial demonstrates using Stereochemistry markers and the flip command.

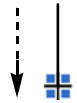
Create a new document.

1. From the **File** menu, choose **New Document**.
2. From the **File** menu, choose **Save As**.
3. Type tut7.cdx in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.

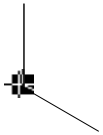
Draw the following structure:



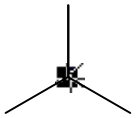
1. Click the Solid Bond tool .
2. Click in the document window and drag downward to create the first bond.



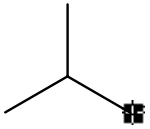
3. Continue pointing at the lower atom and click again to add a second bond.



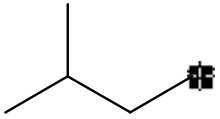
4. Continue pointing at the same atom and click again to add a third bond.



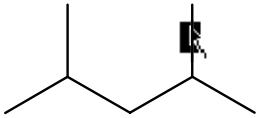
5. Point to the atom shown below and click.



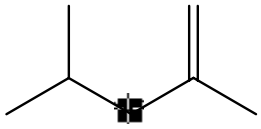
6. Point to the atom shown below and click twice to create two bonds.



7. Pointing to the bond shown below, right-click, point to **Double**, and then choose **Plain**.

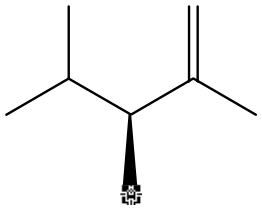


8. Click the Wedged Bond tool, point to the atom below, and then click.

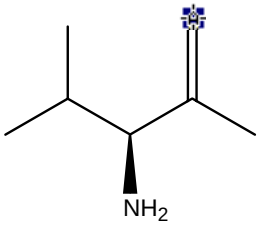


Add atom labels.

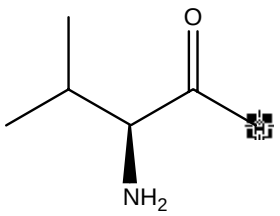
1. With the Text tool, click the atom shown below, and then type NH2 in the text box that appears.



2. With the Text tool, click the atom shown below, and then type O in the text box that appears.



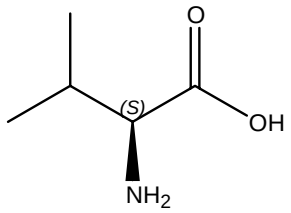
3. With the Text tool, click the atom shown below, and then type OH in the text box that appears.



Display the stereochemical markers.

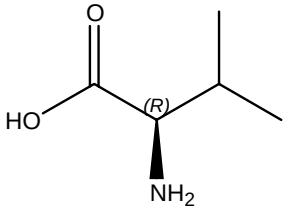
1. Select the entire structure with the Lasso or Marquee.
2. From the **Object** menu, choose **Show Stereochemistry**.

   The S marker appears.



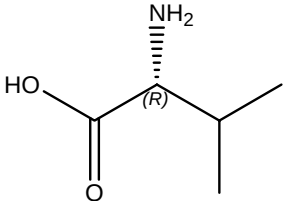
3. Select the structure and from the **Object** menu, choose **Flip Horizontal**.

   The R marker appears.



4. With the structure selected do the following:

   Click the **Object** menu. While holding the mouse button, press the **Alt** or **Shift+Option** key and choose **Rotate 180° Vertical**.



   The Wedged bond becomes hashed and the (R) stereochemistry is preserved.

Save and close the document:

1. From the **File** menu, choose **Save**.
2. From the **File** menu, choose **Close**.

Chapter 3: Drawing Chemical Structures

Overview

ChemDraw provides the following tools for drawing chemical structures:

- Bond tools.
- Ring tools.
- Text tools.
- An acyclic chain tool.
- Automatic error checking.

Drawing Settings

Drawing settings are document settings that affect how bonds and other objects are drawn. You can configure the drawing settings for an entire document or for a particular object as follows:

- For the entire document, use the Document Settings dialog box.
- For an object, use the **Object Settings** dialog box.

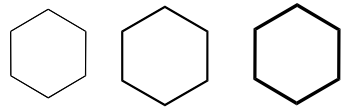
Changes made to the drawing settings affect the active document window only. Drawing settings can be saved in Style Sheets or Stationery Pads.

To apply settings from other documents to your document, select "Apply Document Settings from..." from the File menu.

The drawing settings are described in the following table:

Adjust this...	If you want to ...
Chain Angle	Set the angle (from 1 to 179 degrees) between bonds created by the Acyclic chain tool or modified by the Structure CleanUp command. For more information see, "Drawing Acyclic Chains" on page 68 and *"Using Structure CleanUp" on page 128*.

Adjust this...	If you want to ...
Bond Spacing	Set the distance between the lines in double or triple bonds. The distance is set either as: • The percent of the length of the bond (between 1 and 100). This allows for proportional spacing to be used if different bond lengths are used in the drawing. An absolute value you choose in the units specified for your document.
Fixed Length	Constrain the length of the bonds drawn to the length you specify when the Fixed Lengths command in the Object menu is selected (a check mark is next to it). This also adjusts the preferred bond length for structures modified by the Structure CleanUp command. For more information see "Drawing with Fixed Lengths" on page 64 and *"Using Structure CleanUp" on page 128*.

Adjust this...	If you want to ...
Bold Width	Set the width of the line used when bold and wedge bonds are drawn. The Bold Width setting must be greater than the Line Width setting. The end of a wedge is 1.5 times the bold width.
Line Width	Set the width of all bonds, lines, and arrowheads in the drawing. 
Margin Width	Change the amount of space surrounding all atom labels that will erase portions of the bonds to which they are attached. The margin width also determines the amount of white space surrounding the front bonds in a bond crossing. For more information, see "Editing Atom Labels" on page 87 and "Changing Bond Crossings" on page 71.

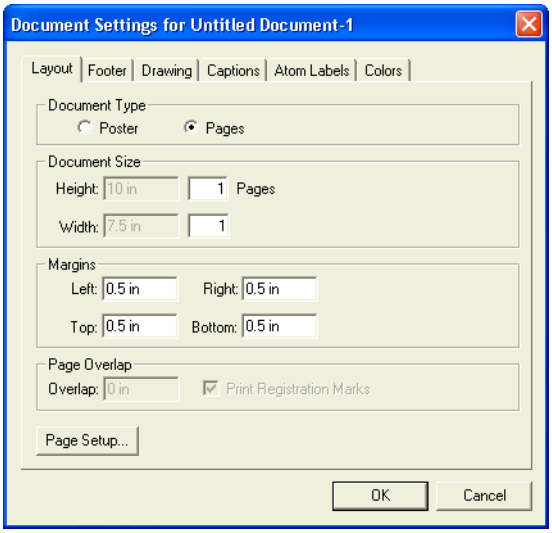
Adjust this...	If you want to ...
Hash Spacing	Set the spacing between the hashed lines used when wedged hashed bonds, hashed bonds, dashed bonds, dashed arrows, or dashed curves are drawn. 2 Point 4 Point 8 Point
Color	Change the color in of selected objects. For more information, see "Customizing the Color Palette" on page 131.
Units	Set the units used in the Object Settings dialog box to centimeters, inches, points, or picas.
Atom and Bond Indicators	Set which indicators you want to display in your drawings. For more information about using indicators, see "Atom Numbering" on page 89 and "Showing Stereochemistry" on page 139.

Configuring Settings for Documents

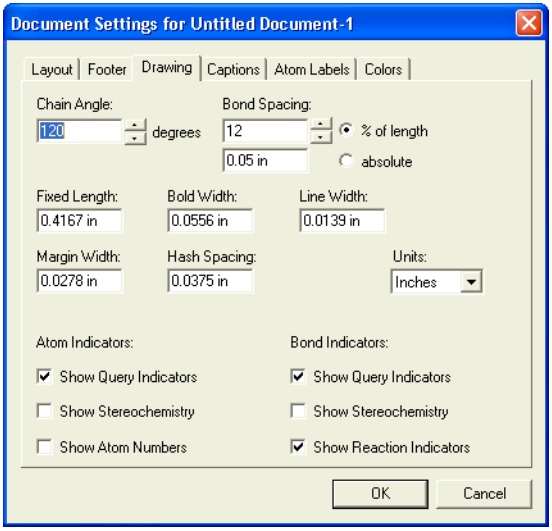
To configure the drawing settings for an entire document:

1. From the **File** menu, choose **Document Settings**.

   The Document settings dialog box appears.



2. Click the **Drawing** tab and configure the settings.



3. Click **OK** when you are finished.

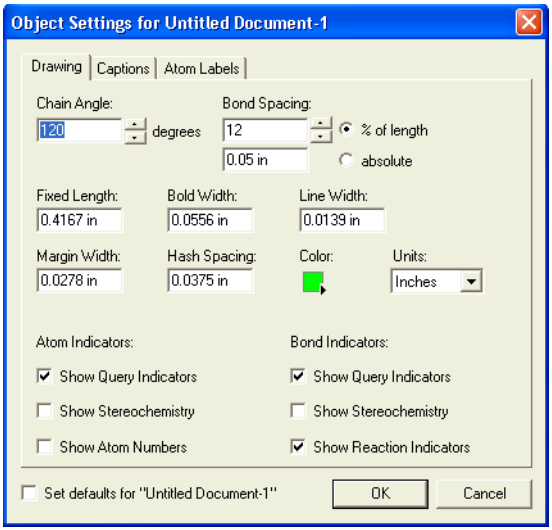
   The settings you chose are applied to the entire document.

Configuring Settings for Objects

To configure the drawing settings for a selected object:

1. Select the object.
2. From the **Object** menu, choose **Object Settings**.

   The Object Settings dialog box appears with the Drawing tab displayed.



3. Configure the settings and click **OK**.

   The settings you chose are applied to the selected object only.

Drawing Bonds

The Main Tools palette contains the bond tools shown below:

Solid Bond

Multiple Bonds

Dashed Bond

Hashed Bond

Hashed Wedged Bond

Bold Bond

Bold Wedged Bond

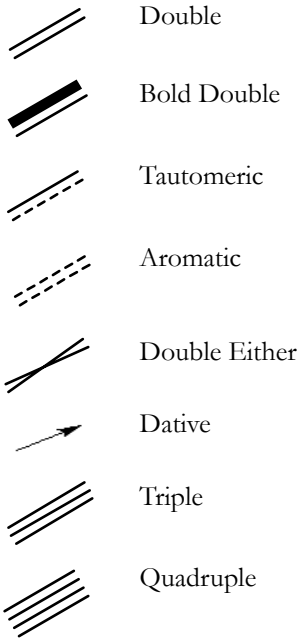
Hollow Wedged Bond

Wavy Bond

Multiple Bonds

The Multiple Bond tool on the Main toolbar includes the following palette.

You can use the tools on the Multiple Bond palette to create the following multiple bonds:



NOTE: *You can also draw multiple bonds by right-clicking over a bond and selecting the bond type from the shortcut menu or by using the bond properties dialog box. For more information, see "Bond Properties" on page 155.*

Double Bonds

There are three ways to draw a double bond:

- Use the Double bond tool
- Using the Solid, Dashed, or Bold bond tool:
  a. click an existing single bond.
  b. drag over the length of an existing single bond.

.Double Either Bonds

To draw a double either bond select the double either bond tool from the Multiple Bonds palette, or:

1. Draw a bond using the Wavy Bond tool.
2. Point to the center of the bond and click to create a double bond
3. Click again to create a double either bond.

Triple Bonds

You can draw a triple bond by drawing another single bond on top of a double bond. All bonds in a triple bond are solid bonds.

To draw a triple bond select the triple bond tool from the Multiple Bonds palette, or:

1. Click any bond tool.
2. Drag from one end of an existing double bond to the other.

Quadruple Bonds

To draw a quadruple bond select the quadruple bond tool from the Multiple Bonds palette, or:

1. Click any bond tool.
2. Drag from one end of an existing triple bond to the other.

   The triple bond changes to a quadruple bond.

To change a quadruple bond into a single bond:

1. Click any bond tool.
2. Drag from one end of an existing quadruple bond to the other.

The quadruple bond changes into a single bond corresponding to the tool used to draw over the bond.

NOTE: *You can also use the Eraser tool to reduce the bond order. For more information, see "Changing the Bond Order" on page 71.*

Drawing Constrained Bonds

You can draw any bond length and create any angle relative to the X-axis. The Info Window displays the bond length and angle as you drag the bond. However, you can draw bonds that are constrained to:

- A fixed length
- A fixed angle relative to the X-axis

Drawing with Fixed Lengths

To draw bonds that are constrained to a fixed length:

1. From the **Object** menu, choose **Fixed Lengths**.

   A check mark appears next to the Fixed Lengths command indicating that it is selected. All the bonds drawn are constrained to the fixed length specified in the Drawing Settings dialog box.
2. Click a bond tool.
3. Drag from one end of the bond to the other.

   The Info Window displays the bond length.

Drawing with Fixed Angles

To draw bonds with constrained angles that are multiples of 15 degrees relative to the X-axis:

1. From the **Object** menu, choose **Fixed Angles**.

   A check mark appears next to the Fixed Angles command indicating that it is on.
2. Click a bond tool.
3. Drag from one end of the bond to the other in a document window.
4. Move the end of the bond to other angles.

   The Info Window shows that the bond angle is constrained to 15-degree increments.

Toggling Fixed Lengths and Fixed Angles

If Fixed Lengths or Fixed Angles are selected, you can temporarily deselect them.

To toggle Fixed Lengths and Fixed Angles:

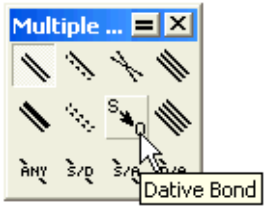
- Press the **Alt** or **Option** key and drag from one end of a bond to the other end in the document window.

Dative Bonds and Wedged Bonds

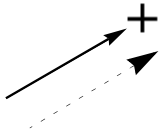
Dative bonds and wedged bonds are drawn with a fixed orientation in a document window.

To draw a dative bond:

1. Click the Dative Bond tool.

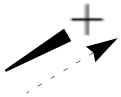


2. Drag from the positive to the negative end (arrow head) of the dative bond.



To draw a wedged bond:

1. Click one of the wedged bond tools.
2. Drag from the narrow end of the wedged bond to the wide end of the wedged bond.



To change the orientation of the dative or wedged bond:

- Click the center of the dative or wedge bond using the appropriate tool.

  The orientation of the bond is inverted.

Adding a Bond by Clicking

To add a fixed length bond:

1. Select a bond tool.
2. Click an atom.

A new bond is drawn and joined to the atom you clicked.

Bonds drawn by this method are always drawn using the Fixed Length specified in the Drawing Settings dialog box. The angle that the deposited bond makes with its nearest neighbor is equal to the Chain Angle set in the Drawing Settings dialog box. If this angle cannot be established, a smaller angle is used.

Adding Bonds by Dragging

To control the orientation of bonds that you draw, you can add bonds by dragging.

By using this dragging method for drawing the bond, you can control the orientation of the other end of the bond.

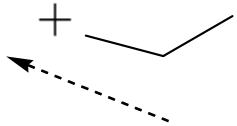
To add a bond by dragging:

1. Click a bond tool.
2. Point to an atom.

A highlight box appears over the atom indicating where the bond will be joined.

3. Drag from the atom at which you are pointing to the end of the new bond.

   A new bond is drawn and joined to the atom where the highlight box appeared.



Changing the Highlight Box Size

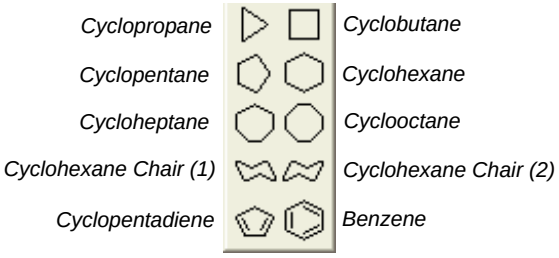
The size of highlight box is controlled by the Tolerance value in the Preferences dialog box. With the default Tolerance setting of 5 pixels, the highlight box appears on atoms if the pointer is located in a square region 10 pixels on a side or +/- 5 pixels from the atom.

To change the Tolerance:

1. From the **File** menu, choose **Preferences**.
2. On the **General** tab, select or type the tolerance, and then click **OK**.

Drawing Rings

The Main Tools palette contains the following ring tools that enable you to draw ring sizes and types:



Drawing a Ring

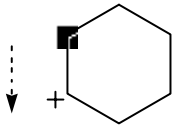
If Fixed Lengths is on when you draw a ring, the length of each bond in the ring is automatically set to the fixed length. If Fixed Angles is on, the angle the first bond in the ring makes with the X-axis is restricted to 15-degree increments. For more information, see "Drawing Constrained Bonds" on page 64.

To draw a ring:

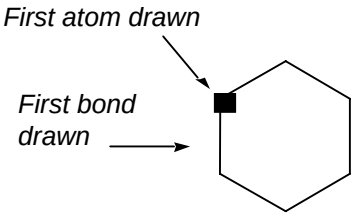
1. Click a ring tool.
2. Position the pointer in a document window.

   The cyclohexane tool is shown below:

3. Drag from the beginning to the end of the first bond.



When you point in a document window, the pointer changes to a ring tool pointer. The highlight box on the ring tool pointer indicates the atom that is drawn first. The bond directly below the highlight box is the bond that is drawn first.



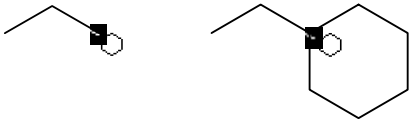
Drawing a Ring by Clicking

To quickly draw a ring:

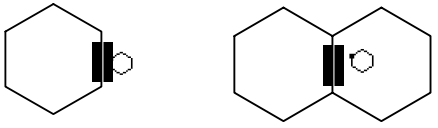
- Click a ring tool, and then click in a document window.

  A ring appears in a document window centered around the pointer. The ring is drawn using the Fixed Length specified in the Drawing Settings dialog box. The ring is deposited in the orientation shown on the ring tool icon.

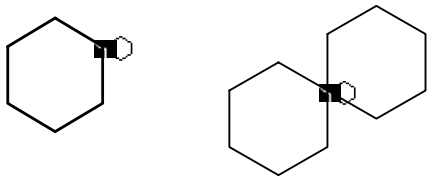
If you click an atom, the ring is fused to that atom.



If you click a bond, the ring is fused to that bond.



If you click an atom in a ring, a spiro linkage is formed.

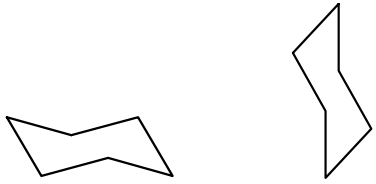


Drawing Cyclohexane Chair Rings

You can draw Cyclohexane chair rings in two orientations: horizontal and vertical.When you draw a cyclohexane chair ring by clicking, the chair is drawn in a horizontal orientation.

To orient a cyclohexane chair ring to a vertical orientation:

1. Click one of the Cyclohexane Chair Ring tools.
2. Drag in the structure to the orientation you want.



Horizontal Orientation *Vertical Orientation*

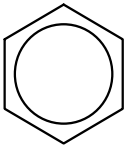
Drawing Resonance Delocalized Rings

Any of the ring tools, except the cyclohexane chairs, can be drawn in a resonance delocalized form.

To draw a resonance delocalized ring:

1. Click a ring tool.
2. Press the **Ctrl** or **Command key** and drag or click to draw the ring.

A circle appears inside the ring.



NOTE: *The circle is automatically grouped with the ring when drawn. For more information on grouping objects, see "Grouping Objects" on page 118.*

Drawing Cyclopentadiene and Benzene Rings

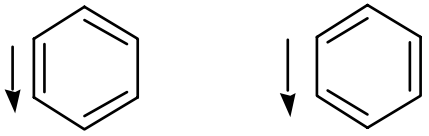
The double bonds in the cyclopentadiene or benzene ring tools can be drawn in either of two forms.

When you draw a cyclopentadiene or benzene ring a double bond is drawn first. The Cyclopentadiene and Benzene Ring tool pointers indicate this orientation.

To shift the orientation so the first bond drawn is a single bond, do one of the following:

- **Shift+drag** from the beginning of the first single bond to the end of the single bond.
- **Shift+click** in a document window to draw the bond with a Fixed Length.

In the figure below, the arrow indicates the direction in which the first bond is drawn.



Drawing Acyclic Chains

You can draw long hydrocarbon chains with the Acyclic Chain tool . The behavior of the Acyclic Chain tool is affected by the "Fixed Lengths" and "Fixed Angles" switches on the Object menu, and by the "Chain Angle" setting on the Object Settings dialog box.

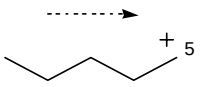
NOTE: *Modifying the Chain Angle value for an existing object will have no effect on that object, but new bonds/chains sprouted from it will sprout at the specified angle.*

The effect of "Fixed Lengths" and "Fixed Angles" is noted in the specific sections where it applies.

Drawing Chains

To draw an acyclic chain:

1. Click the Acyclic Chain tool.
2. Drag in the direction you want the chain to grow in a document window.



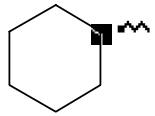
A number appears at the end of the chain indicating how many atoms you have drawn.

When Fixed Lengths is on, the pointer on the acyclic chain can be dragged to make any angle relative to the X-axis. At a constant chain length, the positions of the first bond and all subsequent odd-numbered atoms depend on the direction you drag. Before releasing the mouse button, this position can be changed by dragging in the opposite direction. When Fixed Angles is on, the angle the acyclic chain makes relative to the X-axis is constrained to 15-degree increments.

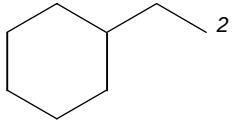
Adding Chains

To add an acyclic chain to an existing atom:

1. Click the Acyclic Chain tool.
2. Point to the atom to which you want to attach the chain.



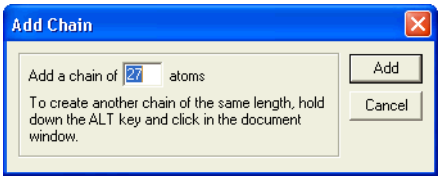
3. Drag in the direction you want the chain to grow.



To specify a chain length:

1. Click the Acyclic Chain tool.
2. Click an existing atom or an empty area in a document window.

   The Add Chain dialog box appears.


Add Chain
Add a chain of 27 atoms
To create another chain of the same length, hold down the ALT key and click in the document window.
Add
Cancel

3. Type the number of bonds in the chain.
4. Click **Add**.

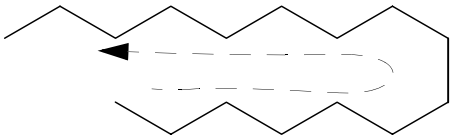
To add another chain of the same length anywhere in a document window:

- **Alt+click** or **Option+click** an existing atom or click in an empty area within the document window.

Changing Chain Direction

To change the direction of the chain as you draw:

- Press the **Ctrl** or **Command** key while drawing chains in the direction you want.



NOTE: *If Fixed Lengths is off, use* ***Ctrl+Alt*** *or* ***Command+Option*** *to reverse chain direction. Fixed Angles must be on to reverse direction.*

Editing Bonds

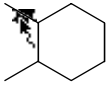
You can modify the appearance of chemical structures by:

- Changing bond types
- Changing bond alignment and orientation
- Moving atoms
- Layering bonds
- Changing the bond order

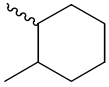
Changing Bond Types

To change a single bond from one type to another:

1. Click a bond tool.
2. Point at the center of an existing bond and click.



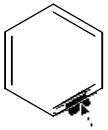
The bond that you click changes to the new bond type.



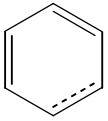
Changing Double Bonds

To change one type of double bond to another:

1. Click the Bold, Dashed, or Solid Bond tool.
2. Point to one of the bonds in the double bond.



3. Click the bond.



The double bond changes to the new bond type. One of the bonds in the double bond is always a solid or dashed bond.

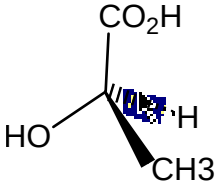
NOTE: *If you click a tautomeric bond (solid/dashed) a second time with the dashed bond tool, you create an aromatic double bond (dashed/dashed).*

Changing Orientation of Wedged and Dative Bonds

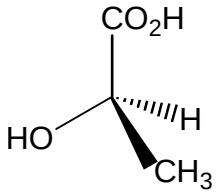
When you draw or change a bond to a wedged or dative bond, the orientation of the bond is chosen appropriately.

To change the orientation:

- Click the dative or wedged bond with the tool used to create it.

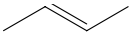
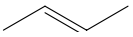
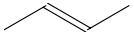


The dative or wedged bond is changed to the opposite orientation.



Changing Alignment of Double Bonds

The bonds in a double bond can have any one of three alignments relative to other bonds:

- Above 
- Below 
- Centered 

To change the alignment of a double bond:

1. Click the bond tool used to create the existing double bond.
2. Do one of the following:
   - Click the center of the double bond.

     The alignment changes. Click the center of the double bond again to change to the next alignment.
   - Right-click or Control-click, point to **Bond Position**, and then choose the alignment.

You may also use Hotkeys to change the alignment:

1. Click a bond or selection tool.
2. Point to the bond and type:

Hotkey	Result
c	to center a double bond.
l	to position a double bond to the left (above).
r	to position a double bond to the right (below).

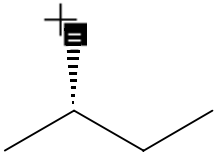
Moving Atoms

You can use any of the bond tools to move an atom within acyclic or cyclic structures. You cannot use a ring tool.

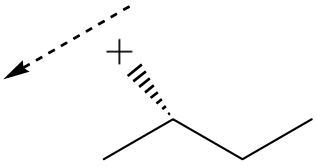
To move an atom in a chemical structure:

1. Click a bond tool.
2. Point at the atom to move.

   A highlight box appears over the atom.



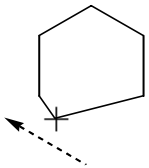
3. Shift+drag the atom.



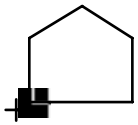
You can convert ring types by dragging one atom on top of an adjacent atom. For example, you can use this method if you want to convert a 6-membered ring into a 5-membered ring.

To convert ring types:

1. With a bond tool selected, point to an atom and **Shift+Drag**.



2. Release when one atom is on top of the other.



The bond between the atoms disappears.

NOTE: *You can also move atoms using a selection tool. For more information see "Moving Objects" on page 111.*

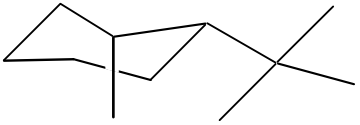
Changing Bond Crossings

When one bond crosses another, white space is used to indicate which bond is in front of the other.

To change which bond is in front:

1. Click any bond tool.
2. Double-click the bond to bring it to the front.

The bond appears in front.



You can also layer bonds using the Bring to Front and Send to Back commands. For more information, see "Front to Back Ordering" on page 185. Another way to layer bonds is to use the Hotkey "f".

NOTE: *You can magnify your view to make changing the bond layering easier. For more information, see "Changing Perspectives" on page 181*

Changing the Bond Order

You can reduce or increase the order of bonds in a structure by using the Bond Properties dialog box or with the shortcut menus as follows.

To reduce the bond order:

1. Point to the bond to change and Right-click or Control-click.
2. Choose the appropriate bond type from the shortcut menu that appears.

To use the eraser tool to reduce the bond order:

1. Click the Eraser tool.
2. Click a single, double, or triple bond.

   The bond order is reduced by one.

To change the bond order using Hotkeys:

1. Click a selection tool.
2. Point to a bond.
3. Type a number from 1 to 4 to change the order.

Automatic Warnings

ChemDraw automatically checks for correct chemical syntax as you draw. If ChemDraw finds a potential problem, a wavy red box is displayed around the questionable object. The red box is displayed on screen only and does not print.

To enable the automatic display of chemical warnings:

- On the View menu, choose **Show Chemical Warnings**.

  This setting applies to all documents.

To view a description of the problem, do one of the following:

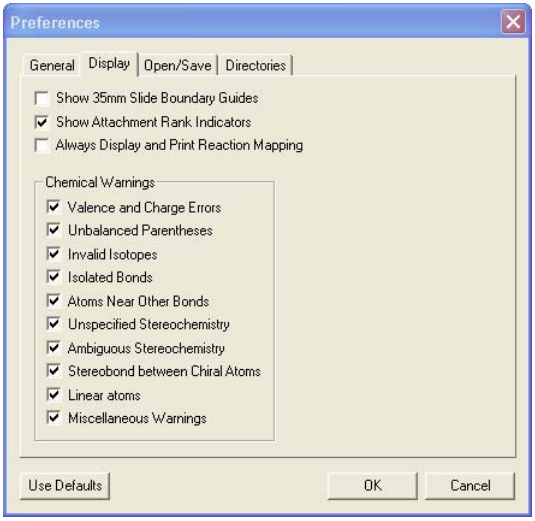
- Point at the warning with the mouse to display a tool tip that describes the error.
- Right-click on the warning and choose **Explain This Warning**.
- Select the structure, and choose **Check Structure** from the Structure menu.

  For more information, see "Checking Chemistry" on page 137.

To select which types of chemical warnings to display:

1. From the **File** menu, choose **Preferences**.
2. Click **Display**.

   The Display tab appears.



3. In the Chemical Warnings section, click the types of warnings you want to display.

To disable the automatic error checking on a specific object:

- Right-click the object and deselect **Display Warnings**.

When Display Warnings is deselected for an object:

- Red boxes are not displayed for questionable objects.
- Problems *are* reported by the Check Structure command. For more information on the Check Structure commands, see "Check Structure" on page 137.

Chapter 4: Ultra Struct<=>Name

Struct<=>Name is CambridgeSoft's package of structure-to-name and name-to-structure algorithms included with ChemDraw Ultra. Together, they give you unprecedented power and convenience in creating and naming structures.

Struct=Name generates systematic names for chemical structures with support for the Cahn-Ingold-Prelog rules for stereochemistry. It is under continuing development to improve the range of compounds covered.

Name=Struct is a comprehensive algorithm for converting English chemical names into chemical structure diagrams. It is designed to interpret chemical names as they are actually used by chemists. In other words, it recognizes the shorthand and slang of everyday usage, in addition to recognizing most of the official IUPAC, IUBMB, and CAS rules and recommendations. In addition, it has an extensive algorithm for the identification of common "typos" (typing errors, such as "mehtyl") to increase the odds of generating structures for the names it is given.

Struct=Name

You can insert the name of a selected structure as a caption using the **Convert Structure to Name** command from the **Structure** menu.

The Struct=Name algorithm in use since ChemDraw 8.0 is a new proprietary naming algorithm developed by CambridgeSoft. It replaces Beilstein's AutoNom algorithm used in earlier versions of ChemDraw. In ChemDraw 9.0, an auto-update feature has been added that renames the structure as you modify it.

The conversion of a structure to a name is limited by many factors. Specifically, Struct=Name makes little or no attempt to name the following:

- Bridged ring systems with more than one bridge (for example, tricycles.)
- Radicals.
- Compounds with non-standard valence states.
- Spiro ring systems.
- Isotopically modified compounds.
- Polymers.
- Biochemicals. including specialized nomenclature for amino acids, carbohydrates, and steroids. For such compounds, only the fully systematic organic name is produced.

Nomenclature types added in ChemDraw 9.0 include:

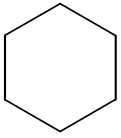
- Most of the most-common fused ring systems, both those with trivial names (naphthalene, indole) and those with systematic names (benzo[e][1,4]diazepine, thieno[3,2-b]thiophene).
- Most salts.
- Structures with a net charge.
- Simple mixtures and multicomponent systems.
- Heterochains.
- Multiplicative nomenclature.
- Ring assemblies.
- Bicyclics.
- Basic inorganics.

Struct=Name generates names with proper CIP stereochemistry descriptors. It has no theoretical limits to the size of the structures that can be named.

To insert the name of a structure into your drawing:

1. Select the drawing for which you want to insert a name.

2. From the **Structure** menu, choose **Convert Structure to Name**.



Cyclohexane

The name of the structure appears as a caption under your drawing.

Auto Update

ChemDraw 9.0 captions include an auto-update feature. Data, including the chemical name and analysis, can be included in a caption, and will update automatically when you modify the structure. For more information on adding data to captions, see "Adding Analysis Data to a Caption" on page 85.

To toggle the auto-update feature:

1. Point to the label.
2. Right-click and select **Auto-update**.

   A check mark appears next to the command when it is selected. Successive clicks toggle the command on and off.

When auto-update is on (default) the label updates each time you modify the structure.

NOTE: *For large complex structures, it may take the new label a few seconds to appear on the screen, depending on the speed of your processor. You do not have to wait for the new label to appear before continuing to modify your structure.*

Name=Struct

You can draw a structure automatically from a chemical name using Name=Struct.

Name=Struct recognizes most organic nomenclature. Inorganic chemistry is also usually recognized, especially when the rules closely match those for organic chemistry.

The following are not supported:

- Coordination complexes
- Polyboranes
- Polymers
- Some highly-bridged ring systems, including fullerenes and porphyrins/porphines
- Some stereochemistry designators: +, -, +/-, +-, D, L, DL, *endo, exo, syn, anti, r, t, c*

Although some trade names are supported, Name=Struct is not intended to interpret trade or common names. A chemical database, such as chemfinder.com, is more appropriate for obtaining structures for trade or common names. See "Finding Information on ChemFinder.com" on page 222 for more information.

NOTE: *Because the syntax of German is very similar to that of English, Name=Struct can also interpret many German names. Chemical names in other languages, however, will generally not be recognized.*

Converting Names to Structures

There are two ways to insert a name into the document window as a structure:

- Insert Structure dialog box
- Paste Special command

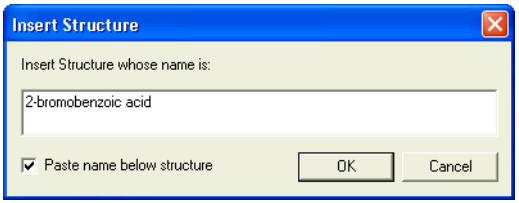
Insert Structure

Insert Structure is designed for typed-in entries. For example, to insert 2-bromobenzoic acid:

1. Choose **Convert Name to Structure** from the **Structure** menu.

   The Insert Structure dialog box appears.

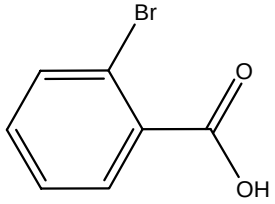
2. Type 2-bromobenzoic acid.



NOTE: *You can also copy a name to the clipboard and then type Crtl+V or Command+V to paste the name into the dialog box.*

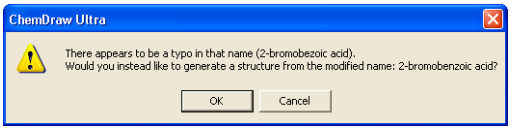
3. Click **OK**.

   The molecular structure and name (if "Paste name below structure" is selected) appear in the drawing area.



2-bromobenzoic acid

If you should happen to type the name incorrectly, Insert Structure will try to correct the error.


ChemDraw Ultra
There appears to be a typo in that name (2-bromobezoic acid).
Would you instead like to generate a structure from the modified name: 2-bromobenzoic acid?
OK
Cancel

Click **OK** to accept the suggested spelling, or click **Cancel** and start again to make a manual correction.

Paste Special

The **Paste Special** command allows you to paste a name, copied to the clipboard from another application, as a structure in ChemDraw.

To paste a name from the clipboard:

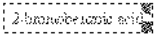
1. Click in the document window.
2. From the **Edit** menu, point to **Paste Special**, and then choose **Name as Structure**.

   The structure appears in your document.

Converting Captions to Structures

If a caption is already present in the drawing area you can convert it to a structure as follows:

1. Select the caption.



2. Choose **Convert Name to Structure** from the **Structure** menu.

   The molecular structure and name appear in the drawing area.

Types of Structures Supported by Struct=Name

Struct=Name can name compounds in the following classes of structures:

category	ChemDraw 8 supports...	ChemDraw 9 adds...
principal groups in both rings and chains	Acid Halides	Amide derivatives of acids
	Alcohols and chalcogen analogs	Anhydrides
	Aldehydes and chalcogen analogs	Carbonic acids
	Amides	Imides
	Amines and Imines	Nitric acids
	Carboxylic Acids	Peroxy acids
	Carboxylic Esters	Salts
	Heteroatomic acid halides	Sulfides and chalcogen analogs
	Heteroatomic acids (P, B, As)	Sulfoxides and chalcogen analogs
	Heteroatomic esters	
	Hydrazides	
	Hydrazines	
	Hydroperoxides	
	Ketones and chalcogen analogs	
	Nitriles	

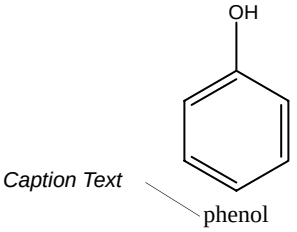
category	ChemDraw 8 supports...	ChemDraw 9 adds...
	Peroxides	
	S, Se and Te Amides	
	S, Se, and Te Acid Halides	
	S, Se, and Te Acids	
	S, Se, and Te Esters	
Ringed structures	Carbomonocyclic structures	Bridged monocyclic structures
	Heteromonocyclic structures	
	Fused polycyclic trivially-named structures	
	Ring fusions of only two rings	
	Ring fusions of two multiple ring systems	
Other compounds		Phosphorous and Arsenic compounds
		Si, Ge, Sn, and Pb compounds
		Boron compounds
		Organometallic compounds

Chapter 5: Drawing Captions and Atom Labels

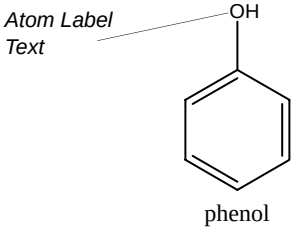
Creating Text

ChemDraw enables you to create the following types of text:

- **Caption text**—Create annotations, chemical names, chemical formulas, page titles, and information in tables.



- **Atom label text**—Identify atoms and substructures by their chemical symbols and formulas.



The behavior of atom labels is controlled by the **Automatic Atom Labels** checkbox on the **General** tab of the **Preferences** dialog box. This preference controls two aspects of the behavior of atom labels. The default preference is to use Automatic Atom Labels.

When Automatic Atom Labels is selected:

- The alignment of atom labels will adjust according to the positions of any bonds attached to the atom label.

  For example, a CH_3 atom label entered at the *left* end of a horizontal bond would reverse itself to H_3C.
- Hydrogens will be added to or removed from atom labels as necessary to preserve standard valences when bonds are added or changed.

You can use HotKeys to quickly label atoms. For more information see "Labeling Atoms with HotKeys" on page 87.

You create and edit caption and atom label text with the Text tool. You set the text format in the Document Settings or Object Settings dialog box.

ChemDraw does not install its own fonts. If a ChemDraw document contains fonts that are not available on a particular computer, they are substituted with available fonts.

Creating a New Line and Closing Text Boxes

The default way to create a new line in a caption text box is with the **Enter** or **Return** key. The default way to create a new line in an atom label is with **Alt+Enter** or **Option+Return**. To close the text box, click outside the text box or select another tool.

To change the default do the following:

1. From the **File** menu, choose **Preferences**.

NOTE: *In Mac OS X, the Preferences dialog box is found on the ChemDraw menu.*

2. On the **General** tab, choose the appropriate option:

To change the default for ...	Select ...
Atom Label text	Require Alt+Enter or Option+Return to Create New Line in Atom Labels.
Caption text	Require Alt+Enter or Option+Return to Create New Line in Captions.

3. Click **OK**.

Formatting Text

Text settings affect how captions and atom labels for the current document are drawn and formatted. Formatting options include:

- Font (font type)
- Size (font size)
- Style (font and baseline style)
- Line spacing
- Alignment

These options are described in the following sections.

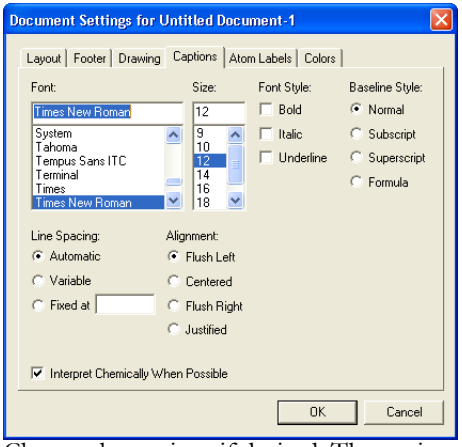
Setting Font parameters

Changing text formats in the Document Settings dialog box affects the current document only. You can also change settings for individual objects by using the Object Settings dialog box, the Text menu, or the Style toolbar.

To edit the document text settings for captions and atom labels:

1. From the **File** menu, choose **Document Settings**.
2. In the **Document Settings** dialog box, click **Captions** or **Atom Labels**.

   The Windows Captions tab containing the text settings is shown below.



3. Change the settings if desired. The options are described in the following sections.
4. Click **OK**.

   The formatting is applied to the current document.

Setting the Baseline Style

You can specify the following baseline styles:

- **Normal—**Use this for standard text.
- **Superscript—**Reduces the text size by about 25 percent and raises its baseline.

- **Subscript—**Reduces the text by about 25 percent and lowers the baseline.
- **Formula—**Formats in a way that is appropriate for most chemical formulas, that is, numbers are automatically subscripted. You must, however, captitalize manually.

You can apply several styles to the same selected caption. You can also apply multiple styles to different portions of a single caption.

If the captions you select have more than one style, when you select the text with the Lasso or Marquee tool and select **Style** from the **Text** menu, a hyphen appears next to each style (other than Plain) that is applied to a portion of the selection. A check mark appears next to each style that applies to all of the selected text. Choosing a style other than "Plain" adds the new style to all of the selected captions. Previously applied styles are not affected—that is, for example, if you select Italic for a section that is Bold, it will be Bold Italic.

Specifying Line Spacing

You can specify the three types of line spacing:

- **Automatic—**Consistently spaced lines of text based on the height of the tallest character in the entire caption. This is the default line spacing.
- **Variable—**Lines of text with different spacing based on the tallest character and the lowest descender in each line.
- **Fixed—**Consistently spaced lines using a spacing that you specify.

Aligning Text

You can set the alignment of captions and atom labels to justify text to suit your needs. The options available depend on whether you are aligning captions or atom labels. Settings are made in the Object Settings dialog box.

To open the object settings dialog box, do the following:

1. Select a caption or atom label with the Lasso or Marquee tool.
2. On the **Object** menu, click **Object Settings**.

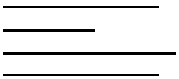
   The Object Settings dialog box appears.

Captions

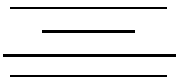
You specify the caption justification and line spacing on the Captions tab of the Object Settings dialog box. All text in a single caption must have the same Justification and Line Spacing.

There are four available justifications:

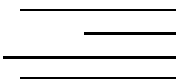
- **Flush Left—**creates left-justified caption text.



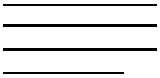
- **Centered—**creates centered caption text.



- **Flush Right—**creates right-justified caption text.



- **Justified—**creates right-left justified caption text.



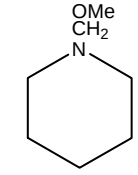
Atom Labels

Use the **Centered**, **Flush Left**, **Flush Right**, **Stacked Above**, or **Automatic** justifications to create labels that identify atoms and functional groups in your chemical structure without obscuring any bonds or other atom labels.

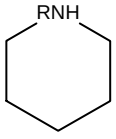
NOTE: *When using Stacked Above justification, enter the tokens from top to bottom using Alt+Enter or Option+Return to go to a new line. For instance, in the example below, enter "OMe Alt+Enter [Option+Return] CH_2 Alt+Enter [Option+Return] N".*

If you change the justification after the label is entered, it will in most cases generate a warning.

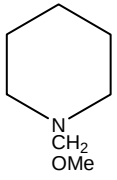
Examples of the atom label justifications are shown below.



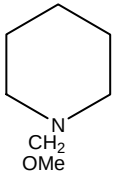
Stacked Above



Centered



Flush Left

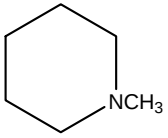


Flush Right

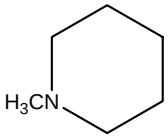
Automatic Alignment

When you justify Atom labels automatically, ChemDraw breaks the label into tokens. A token consists of an uppercase letter followed by any numbers or lowercase letters. The first token is attached to the atom and the rest of the label appears without obscuring other parts of the chemical structure.

For example, to create N-methylpiperidine, label an atom in cyclohexane with the atom label NCH_3, which contains the three tokens, N and C and H_3. If you label C3, the tokens are placed from left to right because there are bonds to the left of the atom.



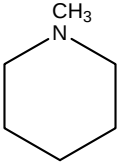
If you label C5, the tokens are placed from right to left because there are bonds to the right of the atom:



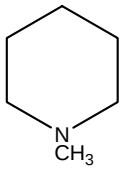
Pro In ChemDraw Pro, you can force an entire multi-atom label to be a token by defining it as a Nickname. This prevents the label from flipping when applied to the left side of a structure.

For example, if you define the Nickname CH_3, and label C5 with the combined label and nickname NCH_3, the final orientation is CH_3N instead of H_3CN. In this case, the Nickname, CH_3, is a token. For more examples, see "Using Nicknames" on page 121.

If you label C1, the second and third tokens are placed above the first token since there are bonds below the atom.



If you label C4, the second and third tokens are placed below the first token.



Changing the Default Caption or Atom Label Text Format

Each new caption or atom label uses default document settings for the font, size, and style of captions and atom labels. You can change the format by:

- Changing the document settings for subsequent drawings in the current document.
- Choosing a new format for an individual caption or label from the Text menu or toolbar before you type.
- Selecting text and applying a new format to an individual label after you type.

Specifying Document Settings for New Text

To specify the text settings for new captions and atom labels in the current document:

1. From the **File** menu, choose **Document Settings**.
2. In the **Document Settings** dialog box, click **Captions** or **Atom Labels**.
3. Click the appropriate options.
4. Click **OK**.

These settings affect all new captions or atom labels in the current document. To use these settings in new documents save them in a Style Sheet or Stationery Pad. For more information, see "Saving Customized Settings as Style Sheets or Stationery Pads" on page 21.

Setting an Individual Text Format Before Typing

You can set the text format for an individual caption or atom label before you type. The format change is applied to the current text only.

To set the text format before you type:

1. Click the **Text** tool and then click in the document window.

   A text box appears.
2. Set the text format in one of the following ways:
   - From the Text menu, choose the format options.
   - From the **Style** toolbar, choose the format options.
3. Type the text in the text box.

   The format is applied to the typed text. Any subsequent text you type is formatted according to the default document settings for the current document.

Changing the Spacing of Individual Text Objects

You can change the text settings for a specific caption or atom. The setting change is applied to the selected object only. You can also choose whether to have the settings applied to the selected text and to all subsequent text you type.

To change the text settings for a specific caption or atom label:

1. Select the text to change with a selection tool.
2. From the Text menu, select the appropriate options.

To change only a part of a single caption you must use the Text tool:

- Select part of the caption with the **Text** tool.

To specify a font and size for selected text, do one of the following:

- Choose the font and size from the **Text** menu.
- Right-click and choose the font and size from the right-click menu.
- From the Style Toolbar, select the font and size from the drop-down menus.

Fractional Character Widths (Macintosh)

On the Macintosh, you can choose to have the spacing between characters as close to proportional as possible. If you are printing to a PostScript printer, this option improves the font appearance.

To set fractional widths:

1. From the **File** menu, choose **Document Settings**.
2. In the **Document Settings** dialog box, click the **Footer** tab.
3. Click **Fractional Widths**.

Coloring Text

You can color captions and atom labels before or after they are typed, and as a whole or in part.

To color a caption or atom label:

1. Select the Text tool.
2. Click in the position where you want to place the text.
3. From the **Color** menu, choose a color.
4. Type the caption or atom label.

To color individual characters:

1. Select part of an existing caption or atom label using the Text tool.
2. From the **Color** menu, choose a color.

NOTE: *Macintosh: Captions that contain multiple colors change to the foreground color when rotated. However, all colors contained in the caption are printed.*

To color several captions or atom labels at once:

1. Select the captions or labels using a selection tool.
2. From the **Color** menu, choose a color.

Creating Captions

The default format options of any new captions you create are specified in the **Captions** tab of the Document Settings dialog box. You may edit these options at any time. The settings affect the current document only.

To create a caption:

1. Click the Text tool .
2. Point in an empty space in a document window.

   A caption text box with a flashing insertion point appears.

3. Type a caption.

   The text box widens as you type to accommodate the caption.
4. To create a new line, press the **Enter** or **Return** key.

5. To close the text box, click outside the text box or select another tool.

NOTE: *You can verify the chemical significance of a caption or atom label using the Check Structure command by selecting it with the Lasso or Marquee tool.*

By default, captions are considered to be chemically significant if possible. For example, if you create a label like CH_3OH, you will be able to attach bonds to it (and it will be modified appropriately) even though you intended it to be a label, not a molecule. Moreover, it's values are included in the Analysis Window, which could be confusing. If you try to label structures "A", "B", and "C", the "B" and "C" labels will be marked with a red box because they have "incorrect valences". To fix this, do the following:

1. Select the label with the Lasso or Marquee tool.
2. Right-click or Control+click in the selection.
3. Deselect the **Interpret Chemically** command.

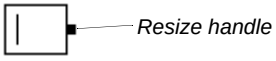
Alternately, you can change the default by unchecking the "Interpret Chemically When Possible" option on the Captions tab of the Document Settings dialog box.

Changing the Caption Width

To change the width of a caption:

1. Select a caption using the Text tool.

   The Caption text box appears around the caption. The right side of the text box contains a Resize handle.



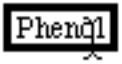
2. Drag the Resize handle.

   The point at which the text wraps is adjusted as you drag the Resize handle.

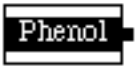
Editing a Caption

To open a caption for editing:

1. Click the Text tool .
2. Point at a caption and click to open the text box.

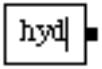


   The caption text is highlighted.



To change all of the highlighted text within an open text box:

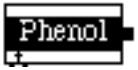
- Type the new caption text over the highlighted text.



   The highlighted text disappears as you type the new caption.

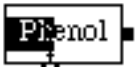
If not all the text is highlighted and you want to select all of the caption text:

- From the **Edit** menu, choose **Select All**.



To change part of the caption text:

- Drag the insertion point over a part of the caption.



Adding Analysis Data to a Caption

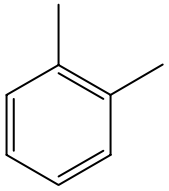
You can add any of the properties from The Analysis Window to a caption. If auto-update is on, the values will update as you modify your structure.

To add values to a Struct=Name label:

1. Point to the label.
2. Right-click, point to **Analysis**, and choose a property from the list.

   The property appears in the label displaying the current value.

NOTE: *You may need to update the window before you can see the new value. If you don't see it immediately, it will appear with the next modification to the structure.*



o-xylene
Chemical Formula: C_8H_{10}
Molecular Weight: 106.16

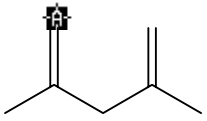
Labeling Atoms with the Text Tool

The default format options of any new atom labels you create are specified in the **Atom Labels** tab of the Document Settings dialog box. You may edit these options at any time. The settings affect the current document only.

To place an atom label on an atom:

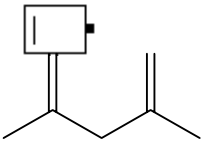
1. Click the Text tool A.
2. Point to an atom.

   The pointer changes when it is positioned correctly over an atom to indicate that you will create an atom label rather than a caption.



3. Click the atom.

   An Atom Label text box appears over the atom.



4. Type an atom label.

   Numbers are automatically subscripted. The justification you choose determines how the letters in an atom label are positioned on a bond. Numbers, leading open parentheses, and trailing closed parentheses are ignored in the positioning of atom labels.
5. To close the text box, click outside the text box or select another tool.

NOTE: *You can use HotKeys to label an atom instead of using the Text tool. You can also label atoms using Nicknames that are text representations of substructures. For more information, see "Labeling Atoms with HotKeys" on page 87 and "Using Nicknames" on page 121.*

Specifying the Margin Width

You can adjust the white space surrounding the atom label so that some of the attached bond is hidden.

To adjust the white space:

1. From the **File** menu, choose **Document Settings**.

   The Document Settings dialog box appears.
2. On the **Drawing** tab, type a new **Margin Width** value.
3. Click **OK**.

4. The margin width is applied to all subsequent drawings in the current document.

Editing Atom Labels

To edit an atom label:

1. Click an existing label using the Text tool or double-click using a bond or ring tool.

   The highlighted atom label text appears within the Atom Label text box.

2. Type the new atom label text over the highlighted text.

If all the text is not highlighted, and you want to select all of the atom label:

- From the **Edit** menu, choose **Select All**.

To edit part of the atom label:

1. Drag the insertion point over part of the atom label.
2. Type the new characters.
3. Close the Atom Label text box.

Deleting an Atom Label

To delete an atom label, leaving the underlying bonds unchanged, do one of the following:

- Click the Eraser tool and then click the atom label.
- With the atom label selected, press the spacebar, Backspace, or Delete Key.

Labeling Atoms with HotKeys

Use HotKeys for rapid labeling of atoms, and applying atom and bond properties. The file **CS ChemDraw Hotkeys** in the ChemDraw Items folder contains the Hotkeys provided with ChemDraw. You can change most Hotkeys, or add new ones, by editing the file in a text editor. (A few are hard-coded. See "Hard-Coded HotKeys" on page 89.) For a list of standard Hotkeys, see "Shortcuts and Hotkeys" on page 247.

TIP: *You can access Hotkey Help directly from the Help menu.*

Use the following methods to label an atom with a Hotkey.

Method 1: Labeling the last atom drawn

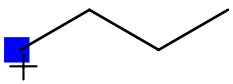
1. Draw a bond by dragging the bond tool in the direction you want the bond oriented.
2. Type a **Hotkey**.

   The last atom drawn is labeled. Each time you draw a bond, the last atom drawn is the Hotkey atom.

NOTE: *When you are pointing, rather than drawing, the last atom highlighted is the atom labeled. Thus, if you click to create a bond and linger with the cursor over the origin, you will highlight the origin and it will be labeled rather than the last atom drawn.*

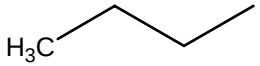
Method 2: Labeling an atom by pointing

1. Using a bond tool or the Text tool, position the pointer over an atom.



   A highlight box appears over the atom.

2. Type a **Hotkey**, for example, c.



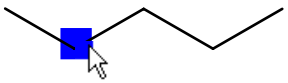
The label is added to the atom highlighted. If the label is a single element, such as C, then the appropriate number of hydrogen atoms are added to the label. Repeatedly typing the hotkey will cycle the number of hydrogens.

NOTE: *The last atom highlighted is always the atom labeled, even if you are no longer pointing to it (that is, even if it is no longer highlighted). This is true even if you switch documents.*

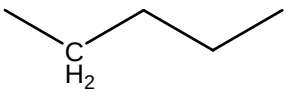
Method 3: Labeling an Atom with a Selection Tool

1. Using a selection tool, position the pointer over an atom.

   A highlight box appears over the atom.

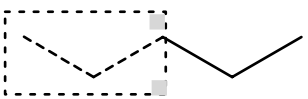


2. Type a **Hotkey**, for example, "c".



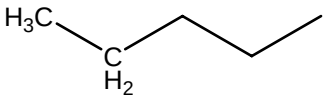
Method 4: Labeling multiple atoms

1. Select several atoms using a selection tool.



2. Type a **Hotkey**, for example, "c".

   The selected atoms are labeled.



The element or label associated with the Hotkey is added to the structure.

Creating HotKeys

To add or edit ChemDraw HotKeys:

Use a text editor (Notepad etc.) to open the CS ChemDraw Hotkeys file in the ChemDraw Items folder.

You can use any uppercase or lowercase alphanumeric key as a Hotkey with the exception of the hard coded HotKeys listed previously. If a capital and lowercase Hotkey do not exist, the Hotkey is assigned to both. If a key is used more than once in the file, the one closer to the end of the file takes precedence.

To add a Hotkey:

1. Add a new line and type the key you want to use.
2. Type a space.
3. Type the letters to associate with the Hotkey.

   HotKeys defined for single elements always result in the adding of the appropriate number of hydrogen atoms.
4. Save and close the HotKeys file.

To create a new HotKeys file:

1. Create a text file named CS ChemDraw Hotkeys.
2. Save the file in the **ChemDraw Items** folder.
3. Click **OK** or **Save**.

Hard-Coded HotKeys

You cannot edit hard-coded HotKeys. The following table contains a list of hard-coded HotKeys:

Hotkey	Function
Enter or **Return**	Opens the atom label text box.
space	Removes an atom label.
Delete or **Backspace**	Deletes objects.

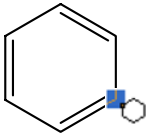
NOTE: *In earlier versions of ChemDraw, quite a few more keys were hard-coded. In ChemDraw 9.0 all keys not listed above can be customized.*

Labeling Atoms With a Bond or Ring Tool

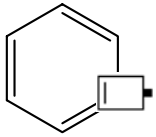
To avoid switching back and forth between tools, you can label atoms with a bond or ring tool.

To label an atom using a bond or ring tool:

1. Click the Bond or Ring tool.
2. Point to an atom and double-click.



An atom text label appears over the atom.



3. Type the text.

Repeating an Atom Label

You can repeat an atom label using the text, bond, or ring tools.

To label several atoms with the same text using the Text tool:

1. Click the Text tool.
2. Label a single atom.
3. Double-click another atom to repeat the previous label.

To label several atoms with the same text using a bond, ring, or Acyclic Chain tool:

1. Click the tool.
2. Triple-click an atom to repeat the previous label.

Atom Numbering

You can add sequential numbering indicators to the atoms in a structure. ChemDraw recognizes the following types of indicators:

- Numbers (1, 2, 3, and so on)
- Text ending with a number (atom1)
- Greek letters in the Symbol font
- Letters (a, b, c, and so on)

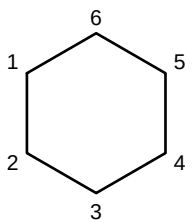
The default indicator is numbers.

Showing and Hiding Atom Numbers

To add Atom Numbering to an entire structure:

1. Select the structure.
2. Do one of the following:

If you want to ...	Then...
show previously assigned atom numbers.	• Right-click, point to **Atom**, and then click **Show Atom Number**. Any previously assigned numbers remain unchanged.
assign new atom numbers.	• Type the Hotkey ' (apostrophe). The atoms in the structure are numbered sequentially.



To number individual atoms

1. Select the atom.
2. Do one of the following:

If you want to ...	Then...
show a previously assigned atom number.	• Right-click, and choose **Show Atom Number**. A previously assigned number is displayed.
assign an atom number	• Type the Hotkey ' (apostrophe). The atoms are numbered in the sequence you choose.

To hide Atom Numbering in a structure:

1. Select the structure.
2. Right-click, point to **Atom**, and then deselect **Show Atom Number**.

To hide an individual atom number, do one of the following:

1. Point to or select the atom, right-click, and then deselect the **Show Atom Number**.
2. Point to or select the atom number, right-click, and then select **Hide Indicator**.

To remove an atom number indicator:

- Click the indicator with the Eraser tool.

Editing Atom Numbers

You can edit the text and style of atom number indicators.

To edit atom number text:

1. Click the **Text** tool.
2. Do one of the following:
   - Select the atom number indicator and type the changes.
   - Double-click the atom number indicator to change to the next character in the sequence.

To edit the atom number style:

- Select the atom number indicator with the Text tool and use the Text menu or Text formatting toolbar.

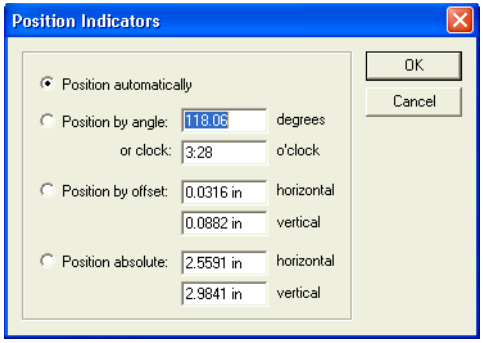
Positioning Atom Number Indicators

Atom number indicators are positioned automatically and move appropriately if a structure is modified. You can reposition them by dragging them to the desired position or with the Position Indicators dialog box.

To reposition an indicator numerically:

1. Right-click the indicator to move and choose **Position**.

   The Position Indicators dialog box appears.



2. Click the appropriate Position option, and type a value:

To position ...	Type a value for Position ...
from the atom or bond center to the indicator center	by angle or by clock
from the atom or bond center to bottom left of indicator baseline	by offset—horizontal and vertical
at specified coordinates	absolute—horizontal and vertical

Typing Non-Roman Text

Use the Character Map for entering non-Roman text, see "Character Map" on page 20. Any font available on the computer can be entered into a label using Character Map.

NOTE: *Two-byte fonts such as Chinese may not work reliably with the Character Map.*

Using the Text Tool with the Lasso Tool

The Text tool used in conjunction with a selection tool enables you to perform additional edits, such as simultaneously changing several captions or atom labels. For more information about selection tools, see Chapter 7: "Manipulating Drawings".

You can toggle between the Text tool and the Lasso tool as follows:

- Press **Ctrl+Alt+Tab** or **Command+Option+Tab**.

  The text box is automatically selected when you switch to the lasso tool.

To switch from the Lasso tool to the Text tool when a caption or atom label is selected:

- Press **Ctrl+Alt+Tab** or **Command+Option+Tab**.

  The Text tool is selected and the text box is opened for editing.

NOTE: *Ctrl+Alt+Tab and Command+Option+Tab will always toggle between the Lasso and last tool used.*

Using Bitmap Fonts When Available (Macintosh)

When text appears in a document on the screen, it can appear using either a bitmap or a TrueType font.

To use bitmap fonts if they are available:

1. From the **File** menu, choose **Preferences**.
2. Select **Use Bitmap Fonts When Available**.

Text drawn using Bitmap fonts looks better and appears more quickly than text drawn using TrueType fonts. However, the size and position of text drawn using Bitmap fonts change somewhat when printed.

For accurate correspondence between what you see on the screen and what is printed:

- Deselect **Use Bitmap Fonts When Available**.

This change affects all documents.

Chapter 6: Drawing Orbitals, Symbols, Arrows, Arcs, and Other Shapes

Overview

ChemDraw provides the following tools and tool palettes that enable you to add chemical symbols and shapes to your documents (A tool palette is indicated by a ▸ in the lower right corner of the tool.):

- **Orbital tools palette** —to draw orbitals.
- **Chemical Symbols tools palette** —to draw charges, radicals, and other symbols.
- **Arrow tools palette** —to draw arrows.
- **Drawing Elements tools palette** —to draw boxes, circles, and lines.
- **Brackets tools palette** —to draw brackets, braces, parentheses, and daggers.
- **Arc tools palette** —to draw arcs.
- **Pen tool** —to draw freehand shapes.
- **TLC tool . to reproduce TLC experiments.**

You can use the tool palettes as extensions of the Main Tool Palette, or you can tear them off and place them anywhere on your screen.

Selecting Tools From a Palette

Some tools have a palette containing different types of that tool. When you choose a tool type from the palette, it becomes the default tool. To use a different tool type, select it.

To select a tool and use its default tool type:

- Click the tool's icon to select it.

To choose a different tool type from the palette:

1. Click the tool's icon and hold down the mouse button.

   The palette appears.
2. Drag to select a tool type from the palette.
3. Release the mouse button over the tool you want to select.

   The selected tool is now displayed on the Main Tools Palette.

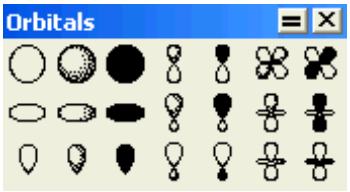
To display a tools palette, do one of the following:

- From the View menu, select **Other Toolbars**, then select one of the palettes.
- Click the tool's icon and drag to the palette's title bar. Release the mouse button over the title bar.

  The selected palette is displayed, and can be dragged anywhere on the screen.

The Orbital Tools Palette

Use the Orbital tools to add orbitals to your chemical structures.



You draw orbitals so that the node appears first. Depending on the orbital type, available fill patterns are:

- Background color
- Shaded
- Solid color

You can modify the fill colors with the Color menu.

Display the Info window to view the orbital's length and angle relative to the X-axis while you draw it. You can constrain the length and angle of an orbital by selecting Fixed Lengths and Fixed Angles on the Object menu.

NOTE: *Orbitals are not normally part of the structure they are drawn near and are not selected when you double-click a bond, atom, or atom label with a selection tool. To group the orbitals with the structure, use the Group command from the Object menu. For more information, see "Grouping Objects" on page 118.*

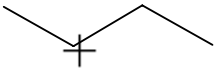
---

s-orbitals

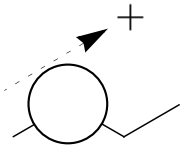
The s-orbital tools are shown below:

To draw an s-orbital:

1. Hold down the mouse button over the Orbital tool and drag to select the **S-orbital** tool from the palette.
2. Point to an atom where the orbital will be centered.



3. Drag outward.

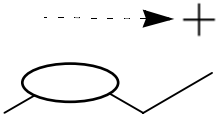


Sigma Orbitals

The σ-orbital tools are shown below:

To draw a σ-orbital:

1. Hold down the mouse button over the Orbital tool and drag to select the **σ-orbital** tool from the palette.
2. Point where the orbital will be centered.
3. Drag outward along the long axis of the orbital.

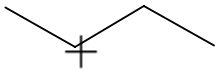


Single Lobe Orbitals

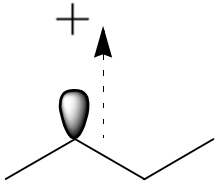
Single lobe orbitals are commonly used for indicating a lone pair. The single lobe orbital tools are shown below:

To draw a single lobe orbital:

1. Hold down the mouse button over the Orbital tool and drag to select the **single lobe orbital** tool from the palette.
2. Point to an atom where the narrow end of the orbital is to be attached.



3. Drag from the narrow end of the lobe to its wide end.

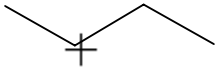


p-orbitals

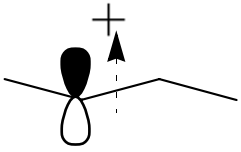
The p-orbital tools are shown below:

To draw a p-orbital:

1. Hold down the mouse button over the Orbital tool and drag to select the **p-orbital** tool from the palette.
2. Point to an atom where the node of the orbital is to be attached.



3. Drag from the orbital node to the wide end of the filled lobe.

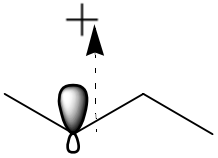


Hybrid Orbitals

The hybrid-orbital tools are shown below:

To draw a hybrid orbital:

1. Hold down the mouse button over the Orbital tool and drag to select the **hybrid-orbital** tool from the palette.
2. Point to an atom where the node of the orbital is to be attached.
3. Drag from the orbital node to the wide end of the major lobe of the orbital.



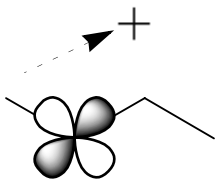
d-orbitals

The d-orbital tools are shown below:

To draw a d-orbital:

1. Hold down the mouse button over the Orbital tool and drag to select the **d-orbital** tool from the palette.
2. Point to an atom where the node of the orbital is to be attached.

3. Drag from the center of the orbital to the wide end of a filled lobe.

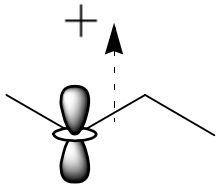


d_{z^2}-orbitals

The d_{z^2} orbital tools are shown below:

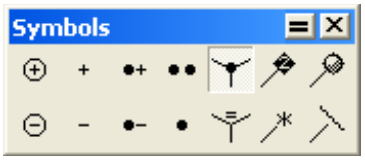
To draw a d_{z^2} orbital:

1. Hold down the mouse button over the Orbital tool and drag to select the **d_{z^2}-orbital** tool from the palette.
2. Point to an atom where the node of the orbital will be attached.
3. Drag from the center of the orbital to the wide end of a lobe.



The Chemical Symbols Tools Palette

Use the Chemical Symbols tools to add chemical symbols to your structure. When you click the Chemical Symbols tool, the following palette appears:



When you attach a symbol (other than H-dot or H-dash) to an atom, it remains at a fixed distance from the central character of the atom label. If you drag the symbol, it will maintain that fixed distance as it moves around the atom.

You can, however, use a symbol without attaching it to an atom, place or move it anywhere, and resize it.

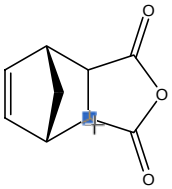
H-dot and H-dash

To represent a hydrogen atom that is coming out of the plane toward you along the Z-axis, use the H-dot symbol .

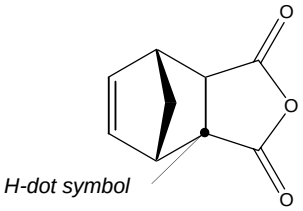
To represent a hydrogen atom that is directed backwards into the plane away from you along the Z-axis, use the H-dash symbol . You can draw H-dots and H-dashes only by clicking atoms.

To draw an H-dot or an H-dash:

1. Hold down the mouse button over the Chemical Symbols tool and drag to select the symbol from the palette.
2. Point to the atom.



3. Click the atom.



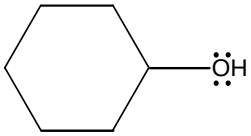
Lone Pair

Use the lone pair symbol to indicate a lone pair of electrons common in Lewis structure representations.

To draw a lone pair:

1. Hold down the mouse button over the Chemical Symbols tool and drag to select the lone pair from the palette.
2. Point to the atom where you want the lone pair located and drag in the appropriate direction to position it.
3. Release the mouse button.

The lone pair is offset from the atom at a fixed position.



To deposit a lone pair symbol in a horizontal orientation:

- Click in a document window.

To change the orientation:

- Click and drag the symbol to the desired orientation.

Radical

Use the radical symbol to indicate a single non-bonded electron.

To draw a radical symbol:

1. Hold down the mouse button over the Chemical Symbols tool and drag to select the radical from the palette.
2. Point to the atom where you want the radical symbol to appear.
3. Click to draw the symbol.

Radical Cation and Radical Anion

Use the charge radical symbols to represent radicals that are charged.

To draw a radical cation or radical anion symbol:

1. Hold down the mouse button over the Chemical Symbols tool and drag to select the symbol from the palette.
2. Point to the atom where you want the symbol to appear.

3. Drag from the charge portion of the symbol to the radical portion of the symbol.

To quickly deposit a radical cation or radical anion symbol in a horizontal orientation:

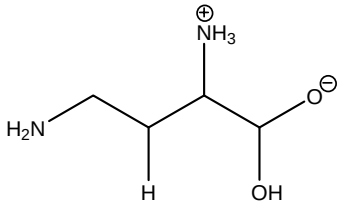
- Click to deposit the symbol.

Charge Symbols

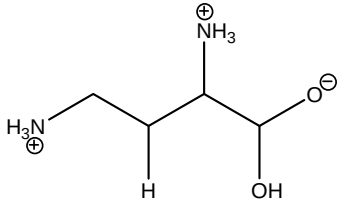
Use the charge symbols to represent charges on structures. + – ⊕ ⊖

To draw a charge and associate it with a structure:

1. Hold down the mouse button over the Chemical Symbols tool and drag to select the charge symbol from the palette.
2. Click to the atom to which you want the charge to correspond.

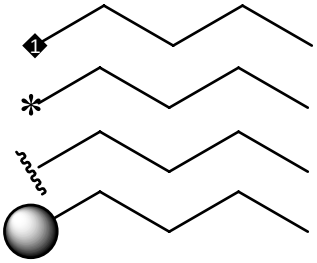


The number of hydrogen atoms increases or decreases as appropriate for the addition of the charge.



Attachment Points

The ability to indicate an attachment point is useful in polymer-bound combinatorial synthesis, protein chemistry, and other situations. ChemDraw has four standard attachment point drawing tools that allow you to indicate a point of attachment while maintaining chemical meaning.



The bead tool is specifically intended to indicate attachment to a resin, but the tools are interchangeable. Any if these tools may be used for variable attachments in queries (see "Using Variable Attachment Positions" on page 127), but only the diamond tool will show rank numbers. That is, if you add more than one diamond to a structure, the points will automatically number sequentially.

Rotating a Symbol

With the exception of the charge and the radical symbols, you can rotate the symbols by selecting and dragging the Rotation handle on the Selection Rectangle. All symbols are rotated around the same end from which they were originally drawn. For example, the radical cation symbol is rotated and resized from the charge. The Info window shows the angle that one of the ends of a symbol makes with the X-axis as you rotate symbols.

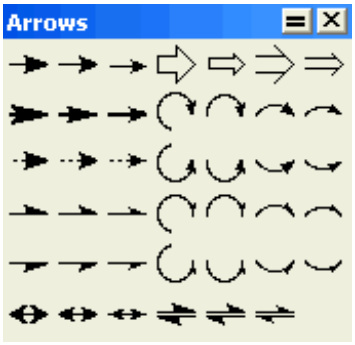
To rotate a chemical symbol:

1. Select the chemical symbol with a selection tool.
2. Drag the Rotation handle on the chemical symbol.

For more information about rotating and resizing, see "Rotating Objects" on page 113.

The Arrow Tools Palette

Use the Arrow tools to add arrows to show the conversion of reactants to products and to indicate electron flow.



NOTE: *Use the Pen tool to make customized arrows. For more information, see "The Pen Tool" on page 102.*

Drawing an Arrow

To draw an arrow:

1. Click the Arrow tool .
2. Point in the document where you want the beginning of the arrow to appear.
3. Drag to where you want the arrowhead to be.

Editing an Arrow

To lengthen, shorten, or rotate an arrow:

1. Click the Arrow tool .
2. Hold down the **Shift** key and point to the head of the arrow.

   A highlight box appears over the head of the arrow.
3. Drag the arrowhead.

The arrow is resized and rotated relative to its end. The Info window shows the change in length and the angle the arrowhead makes with the X-axis as you drag.

You can resize and rotate an arrow using a selection tool by dragging the Resize or Rotation handle on the Selection rectangle (see "Rotating Objects" on page 113 and "Resizing Objects" on page 115). The resize or rotation occurs around the center of the Selection rectangle. The Info window indicates the percentage enlargement or reduction when you drag the Resize handle and the number of degrees rotated when you drag the Rotation handle.

You cannot change the aspect ratio (ratio of height to width) of arrows.

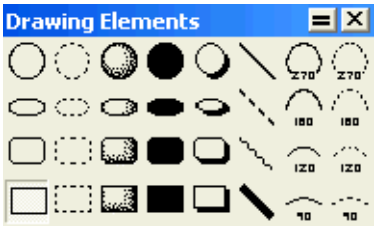
The Drawing Elements Tools Palette

The Drawing Elements tools provides shapes you can add to your drawing.

Drawing elements are not a part of the structure they are drawn near. If you double-click on a bond, atom, or atom label with a drawing tool, they are not selected. To group drawing elements with a structure, use the Group command in the Object menu. For more information, see "Grouping Objects" on page 118.

Some drawing element types are available with fill patterns: hollow (no fill pattern), gray, and black. You can change the type of box, circle, or oval using the Curves menu.

The Info window indicates the length and angle relative to the X-axis while you use any of the drawing element types.



Drawing Boxes

To draw a box:

1. Select one of the box tools.

2. Point where you want a corner of the box to be located.
3. Drag from one corner of the box diagonally to the opposite corner.

Drawing Circles and Ovals

To draw a circle or oval:

1. Select one of the circle or oval tools.

2. Point where you want the center of the circle to be located.
3. Drag outward from the center.

Resizing or Rotating Drawing Elements

A drawing element is resized or rotated from the same point that it was originally drawn. For example, a shadowed box is resized from the corner where the plain edges meet.

You cannot rotate Boxes, Brackets, or Daggers. When a box or closed bracket is rotated along with objects within its borders, the area of the box or closed bracket increases to accommodate the rotation of the contained objects.

To resize or rotate a drawing element:

1. Select the Drawing Element tool.
2. Hold down the **Shift** key and point to an end or edge of a drawing element.

   A highlight box appears.
3. Drag the object to the new size or orientation.

   The Info window shows the percentage enlarged or reduced when you drag the Resize handle and the number of degrees the object rotates when you drag the Rotation handle.

To scale atom labels when resizing:

- Hold the **Control** or **Command** key while dragging to resize.

Distorting Circle and Ovals

You can distort circles and ovals (Shift+dragging the Resize handle) to convert them into an equivalent closed curve. You can distort gray shaded circles and ovals to convert these objects to solid filled curves with fill the same color as the curve. You can also distort boxes and closed brackets.

The remaining Drawing Element types cannot be distorted. For more information, see “Rotating Objects” on page 113 and “Resizing Objects” on page 115.

Drawing Lines

Lines drawn with the line tool differ in two significant ways from bonds drawn with the bond tools:

- They are not included in chemical interpretation of the drawing
- Lines that cross appear solid

To draw using a line tool:

1. Select a line tool.

2. Point where you want the line to start.
3. Drag from one end of the line to the other end.

The Brackets Tools Palette

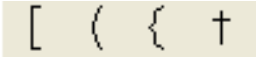
Brackets includes braces {}, brackets [], and parentheses ().

Drawing Single Brackets

A single bracket can be drawn in any orientation.

To draw a single bracket:

1. Select a single bracket tool.



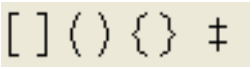
2. Point where you want the bracket to start.
3. Drag from one end of the bracket to the other end.

Drawing Paired Brackets

Paired brackets can only be placed in a vertical orientation. A rectangle or box defines their position.

To draw a paired brackets:

1. Select a paired bracket tool.



2. Point where you want a corner of the bracket to be located.
3. Drag from one corner of the box diagonally to the opposite corner.

Drawing Daggers

To draw a dagger:

1. Select a dagger tool.

2. Point where you want the symbol to be located.
3. Click to deposit the dagger.

NOTE: *The size of the dagger symbol is proportional to the Atom Label font size specified in the Text Settings dialog box.*

Framing Objects

You can enclose your drawings or group structures with a rectangle, brackets, parentheses, or braces.

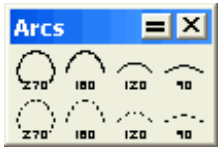
To enclose your object:

1. Select the drawing to enclose.
2. On the **Object** menu, point to **Add Frame**, and then choose the type of frame to add.

The frame you selected is inserted in your drawing.

The Arc Tools Palette

Use the Arc tools to draw solid or dashed arcs of different angles: 90°, 120°, 180°, and 270°.



Drawing Arcs

Where you access the arc tools depends on which version of ChemDraw you are using.

To draw an arc:

1. Do one of the following:
   - In ChemDraw Std, point to the Arc tool and drag in the palette to select the angle.
   - In ChemDraw Pro or Ultra, point to the Drawing Elements tool and drag in the tool palette to select the angle.
2. Dragging from left to right creates a convex arc; from right to left a concave one.

   The Info window shows the length between the ends, and the angle the clockwise end makes with the X-axis while you draw an arc.

Editing Arcs

To resize or rotate an arc using the Arc tool:

1. Select the Arc tool.
2. Hold down the **Shift** key and point to the clockwise end of the arc.

   A highlight box appears.
3. Drag the clockwise end of the arc.

The arc is resized and rotated relative to the end from which it was drawn. The Info window indicates the distance between the ends of the arc and the angle the clockwise end makes with the X-axis.

You can resize and rotate an arc by dragging the Resize or Rotation handle on the Selection rectangle. The resize or rotation occurs around the center defined by the Selection rectangle. When you drag the Resize handle, the Info window indicates the percentage enlarged or reduced. When you drag the Rotation handle, the Info window indicates the degree rotated. For more information, see "Rotating Objects" on page 113 and "Resizing Objects" on page 115.

The Pen Tool

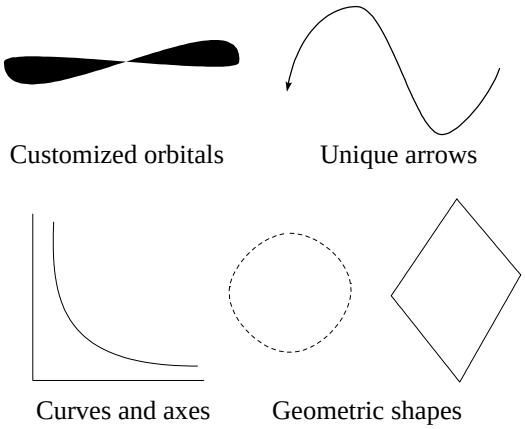
Use the Pen tool to draw shapes that are not provided in the Arrow, Orbital, or Drawing Elements palettes. For example, you can draw irregularly shaped arrows, curves depicting graphs or reaction coordinate diagrams, and other irregularly shaped solids.

The Pen tool has two modes:

- **Drawing**—Used to create shapes. The hand cursor appears with a "+" sign inside.
- **Edit**—Used to edit shapes. The hand cursor appears without a "+" sign inside.

NOTE: To enter edit mode directly from drawing mode, press the **Esc** *key.*

Some examples of shapes that you can draw using the Pen tool are shown below.



To toggle between a selection tool and the Pen tool do one of the following:

- Press **Ctrl+Alt+Tab** or **Command+Option+Tab**
- Click a selection tool.

  The last drawn curve and a selection tool are selected.

Drawing Bézier Curves by Dragging

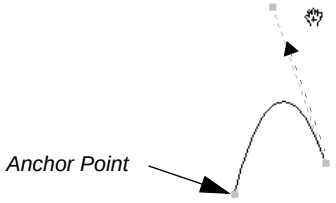
A Bézier curve is a curve that is calculated to connect separate points into a smooth line.You can draw Bézier curves with the Pen tool by clicking and dragging repeatedly to create curved segments.

To draw a Bezier Curve:

1. Select the Pen tool.
2. Point to where you want the beginning of the curve to appear and click.

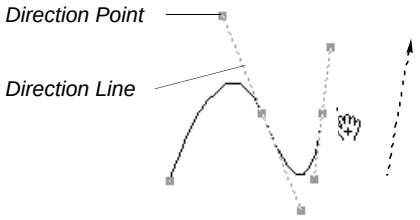
   An anchor point appears, and the cursor changes from a "+" to a hand.
3. Move the cursor to another position and click.

   A line connects the two points.
4. Position the cursor on one of the points (the "+" in the hand will disappear when you are correctly positioned) and drag to create an arc.



A direction line appears tangentially to the curve. Use the direction line to control the "curviness" of the segment. The slope of the direction line determines the slope of the curve. The length of the direction line determines the height of the curve.

Direction points appear at the ends of the direction line. Use the direction points to adjust the curve by dragging a point. You can further adjust the shape by dragging an endpoint of the curve.



Drawing Segments by Clicking

You can draw shapes with corners by clicking repeatedly in an outline of the shape you want.

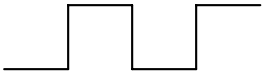
To draw segments:

1. Select the Pen tool.
2. Point to where you want the beginning of the curve to appear.

3. Click to deposit an anchor point.

4. Move the cursor and click again to add a second point.

5. Continue until you have the curve you want.



6. Press the **Esc** key or click another tool.

NOTE: *To place the fewest strategically placed control points for obtaining the smoothest curve, work in a magnified view.*

Editing a Curve

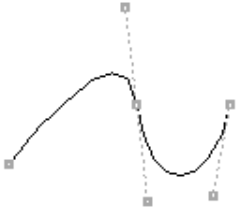
You can edit a curve by selecting it and manipulating it with the direction lines.

To select an existing curve:

1. Select the Pen tool.
2. Point at the curve.

   The cursor will change from a "+" to an arrow when you are positioned correctly.
3. Click to select the curve.

   The direction lines appear.

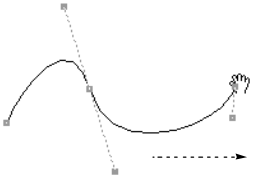


Changing the Shape of a Curve

Use the endpoints of the direction lines to increase or decrease the breadth of the curve or change its direction.

To change the shape of a curve:

1. Select the Pen tool and click the existing curve you want to edit.
2. Drag the direction lines to create the shape you want.



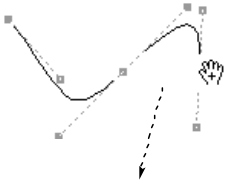
Adding a Segment

To extend an existing curve by adding a segment:

1. Select the Pen tool and click the existing curve you want to edit.
2. Point to the endpoint of a curve until the cursor appears as a hand.

3. **Alt+click** or **Option+click** the endpoint.

   The cursor appears as a hand with a "+" sign inside.



4. Drag to connect more segments to your curve.

Deleting a Segment

To delete a curve segment:

- In the edit mode of the Pen tool, **Alt+Shift+click** or **Option+shift+click** the control point where you want to delete a curve segment.

  The cursor appears as the Eraser tool before you click.

You can also delete entire curves using a selection tool or the Eraser tool.

Applying a Style to a Shape

All curves are drawn with the last curve style chosen until you change the selections. Certain styles are mutually exclusive. For example, if you choose Closed, you cannot also choose Arrow at Start.

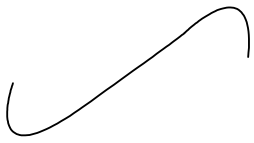
You can use the Doubled style to represent cell membranes. The lines are separated by twice the Bold Width setting for the drawing. Doubled lines cannot be dashed or include arrows.

To apply a style to a curve:

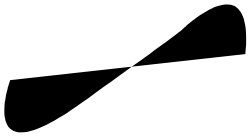
1. Select a curve using either the Pen tool or a selection tool.
2. From the **Curves** menu, choose a style.

Filled and Closed Styles

The illustration below shows a shape with the Plain style applied.



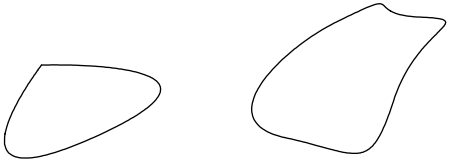
The following illustration shows the shape above with the Filled and Closed styles applied.



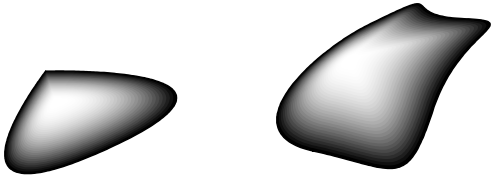
Shaded Style

You can apply shading to any curve, however the shaded style works best with convex or slightly concave shapes. Shading may not appear as desired in extremely concaved shapes.

The illustration below shows shapes with the Plain style applied.



The following illustration shows the above shapes with the Shaded style applied.



Plain Style

To remove all styles from a curve:

- With a curve selected, choose Plain from the Curves menu.

Pro The TLC Tool

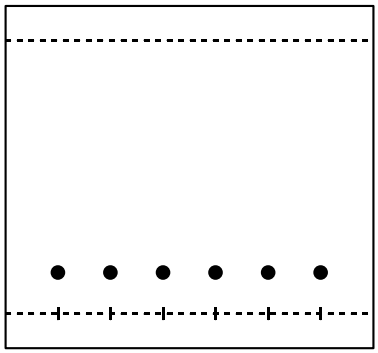
The TLC Tool is a drawing tool that allows you to easily depict Thin Layer Chromatography plates within a ChemDraw document. The tool creates a

rectangular plate with origin line, solvent front, and one or more lanes. The lanes can be populated with spots of different R_f, size, shape, or color.

To create a TLC plate:

1. Select the TLC tool .
2. Drag in any direction from the point of origin.

   The number of lanes is a function of the width of the plate you create.



You can manipulate parts of the plate as follows:

If you want to...	then...
Change the height or width of the plate.	**Drag** a border or corner. The number of lanes will not change.
Move the origin or solvent front.	**Drag** the origin or solvent front line.
Show or hide the origin, solvent front, borders, or side ticks.	1. **Right-click** or **Control-click** in the plate. 2. Select the appropriate action. *NOTE: Use the Transparent option if you want to overlay the TLC plate on a scanned plate.*
Change the order of lanes.	**Drag** the origin tick to the new location.
Add, delete, or duplicate a lane.	1. Position the cursor on the lane you want to delete or duplicate (or between lanes to add). 2. **Right-click** or **Control-click** in the plate. 3. Select the appropriate action. *NOTE: You can also delete lanes with the Eraser tool.*
Move a spot.	**Drag** the spot. The R_f displays as you drag.
Duplicate a spot.	**Ctrl+drag** or **Option+Drag** the spot.

If you want to...	then...
Delete a spot.	Click on the spot with the Eraser tool. *NOTE: If you erase all spots in a lane, the lane will be deleted.*
Display or set the R_f for a spot; add a custom spot	1. **Right-click** or **Control-click** on a spot. 2. Point to **TLC Spots**, and take the appropriate action. *NOTE: To display R_f for all spots,* **Right-click** or **Control-click** *in the plate and select* **Show Rf** *from the TLC Spots submenu.*
Change the style or color of a spot.	1. **Right-click** or **Control-click** on a spot. 2. Choose the style or color. *NOTE: To change the style for all spots,* **Right-click** or **Control-click** *in the plate and choose the style from the TLC Spots submenu.*
TLCEnlarge or "smear" a spot.	**Shift+drag** the spot. When you position the cursor on a spot and press "Shift", the cursor assumes one of three shapes, depending on how it is positioned: 1. Cross arrows . used to enlarge a spot. 2. Horizontal arrow . used to widen a spot. 3. Vertical arrow . used to elongate a spot or create a crescent. *NOTE: You may want to zoom in to make positioning easier.*

R_f Display

When you select Show R_f, a text label appears near the spot showing the spot's retention factor value. By default, the tag will show the R_f to two decimal places. You can change the tag as follows:

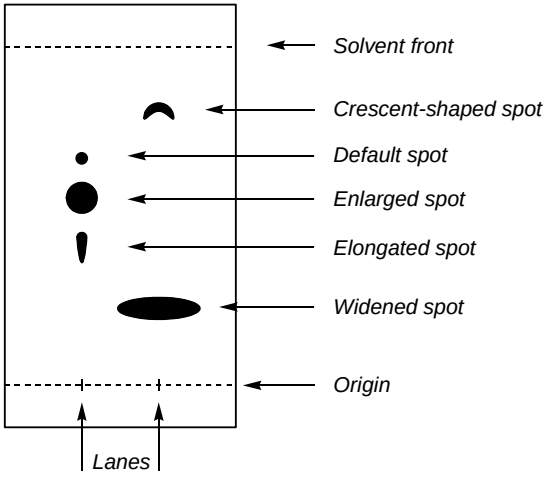
- Select the tag with the Lasso or Marquee tool and drag it to a new location, or **Right-click** or **Control-click** on the tag and choose **Position...**
- Select the tag with the Text tool and edit the R_f value.

  If you change the R_f the spot will move to the new position indicated.

  If you edit the R_f to have different precision, that precision will be preserved.

Resizing Spots

You can resize spots by holding down the Shift key while pointing at an edge of the spot. Dragging the left or right sides of the spot will adjust the spot's width only. Dragging from the top will adjust its height only. Dragging from the bottom will adjust the tail only. Dragging from any of the other four corners will scale all three values. By using combinations of these dragging motions, you can reproduce any sized or shape spot you want.



Custom Spots

The TLC tool can create the most common spot shapes. Other types of spots, such as smears, can be reproduced as custom spots. The **Add Custom Spot** command allows you to insert a graphic file for a spot. Typically, these files would be produced by scanning a TLC plate and saving the spots in a library of spot shapes.

Chapter 7: Manipulating Drawings

Overview

The Lasso or Marquee tools enable you to select objects to edit. You can select objects individually or as groups. You can then duplicate, move, resize, rotate, or delete the selected objects.

Using a Selection Tool

You can use the Lasso or the Marquee selection tool to select all objects. You use the Lasso to select objects freehand and the Marquee to select rectangular regions.

You can set ChemDraw so that the last object drawn to selected when you click the Lasso tool.

To set this option:

1. From the **File** menu, choose **Preferences**.
2. On the **General** tab, select **Automatically Select Recent Objects When Choosing Lasso**.

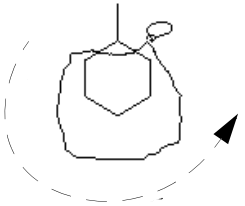
   When you click the Lasso tool, a selection rectangle appears around the last object drawn.

Selecting Objects with the Lasso Tool

Use the Lasso tool to make freehand selection of irregular areas.

To select objects using the Lasso tool:

1. Select the Lasso tool .
2. Press the mouse button while the pointer is not over any object.
3. Drag around a portion of a chemical structure or other object.



As you drag, a line appears which defines the Selection area. Bonds, structures, or other objects are selected only if they are entirely within this area. The end points of the Lasso are automatically connected when you release the mouse button.

Selecting Objects with the Marquee Tool

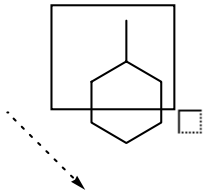
Use the Marquee tool to select objects and structures within a rectangular area.

To select objects using the Marquee tool:

1. Select the Marquee tool .

   The pointer becomes a Marquee.

2. Drag diagonally across the chemical structures or other objects.



As you drag, a rectangle appears which defines the Selection area. Bonds and other objects are selected only if they are entirely within the rectangle.

You can use the Marquee to select several objects at once if they can be surrounded by a rectangle.

Toggling Between Selection Tools

You can set one selection tool to behave like the other as follows:

- Click the Lasso or Marquee tool and press the **Alt** or **Option** key.

Toggling Between Other Tools

To toggle a selection tool and the last drawing tool used:

- Press **Ctrl+Alt+Tab** or **Command+Option+Tab**.

This command will toggle the last selection tool you have used with the last drawing tool you have used. If you haven't used either selection tool, it defaults to the Lasso tool.

Selecting Objects by Clicking

To select an object by clicking:

1. Select the Lasso or the Marquee tool.
2. Point to an object in a document window.

A highlight box appears over the selected object. If you point at a bond, the highlight box appears over the length of the bond.

3. Click the object.

The selected objects appear within the Selection Rectangle and the cursor changes to a hand.

NOTE: *If the bond or other object is part of a group you can select it as an individual object. For more information, see "Grouping Objects" on page 118.*

Setting the Highlight Box Tolerance

You determine the size of the highlight box and how close you must get to activate an object by setting the Tolerance. The standard setting for the Tolerance is 5 pixels. At this setting, the highlight box appears on bonds if the pointer is located 5 pixels or less from any point on the bond.

To set the Tolerance:

1. From the **File** menu, choose **Preferences**.
2. Select or type the tolerance.

   This change affects all documents.

Selecting Entire Structures

To select an entire chemical structure:

- Using a selection tool, double-click a bond or atom within the structure.

The entire chemical structure is selected.

If the chemical structure or other object is part of a group, the entire group is selected. For more information, see "Grouping Objects" on page 118.

Making Multiple Selections

To make multiple selections or add more objects to the selection:

- Press **Shift** and select the other objects.

You can add objects to the Selection by clicking, double-clicking, or by using the selection tools.

Removing Objects from the Selection

To remove an object from the selection:

- Press **Shift** and select an object contained within the Selection rectangle by clicking, double-clicking, or with a selection tool.

  The object is removed from the selection.

NOTE: *Objects may appear within the borders of the Selection rectangle, but not be selected. Only objects that are shimmering are selected.*

Selecting All Objects

To select all objects within a document window:

- From the **Edit** menu, choose **Select All**.

Deselecting All Objects

To deselect all selected objects, do one of the following:

- Click in any empty area in a document window that is outside the Selection rectangle.
- Press **Esc**.
- Select a different tool.
- Select another object without holding down **Shift**.

  The selected objects are deselected.

Deleting Objects

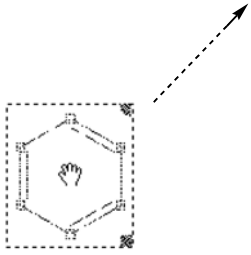
To delete selected objects, do one of the following:

- Press **Delete**.
- Press **Backspace**.
- From the **Edit** menu, choose **Clear**.

Moving Objects

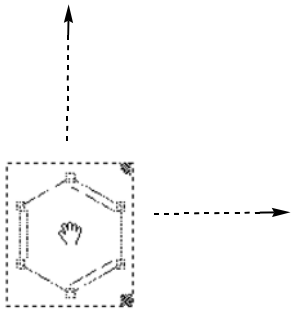
To move an object:

1. Select the object using a selection tool.
2. Point within the border of the Selection rectangle.
3. Click and drag the object.



To constrain the movement to the horizontal or vertical direction:

Shift+drag the selected objects.



Small incremental movements are often useful for aligning objects.To move an object a small distance:

1. Select the object.
2. Press an **arrow** key.

   The selected object moves 1 point in the direction of the arrow.

To move in a larger increment:

Press **Alt or Option** plus an **arrow** key.

The selected objects move 10 points in the direction of the arrow.

For more information about aligning objects, see Chapter 11: "Working With Page Layout".

Using the Clipboard

Use the Clipboard to remove the objects contained in the Selection rectangle for later use. You can paste the copy from the Clipboard to another position in the same document, to another ChemDraw document, or to a different type of document.

Cutting

To use the clipboard:

1. Select the object with a Selection tool.
2. From the **Edit** menu, choose **Cut**.

   The object is transferred to the Clipboard and deleted from a document window.

Pasting

To paste a copy of the contents of the Clipboard into a document window:

1. Click a Selection tool.
2. From the **Edit** menu, choose **Paste**.

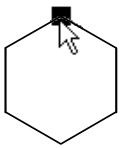
For information about transferring ChemDraw pictures to other types of documents see "Autoscaling" on page 193.

Moving Atoms

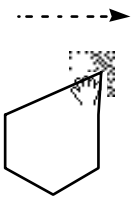
You can move the atoms within a chemical structure using a selection tool.

To move a single atom:

1. Point to an atom using a selection tool.



2. Drag the atom.



   The bonds connected to the atom stretch.

To move multiple atoms:

- Select only the bonds that have atoms on both ends that you want to move.

The unselected bonds that are attached to the selected atoms are stretched.

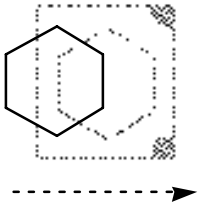
NOTE: *You can also move atoms using the bond tool that was used to draw the atom. For more information, see "Moving Atoms" on page 70.*

Duplicating Objects

To duplicate objects with a selection tool:

1. Click a selection tool.
2. Select the objects.

3. **Ctrl+drag** or **Option+drag** to create a copy and position it.



A copy of the selected objects is moved to the new position.

To duplicate the selected objects and constrain the positioning of the copy to the same position as the original objects:

1. Select a selection tool.
2. Select the objects.
3. **Ctrl+Shift+drag** or **Option+Shift+drag** to create a copy and position it.

To place a copy of an object on the Clipboard:

1. Select the objects using a selection tool.
2. From the **Edit** menu, choose **Copy**.

A copy of the object is placed on the Clipboard.

You can transfer the copy on the Clipboard by the pasting it to the current document, another ChemDraw document, or a different document type.

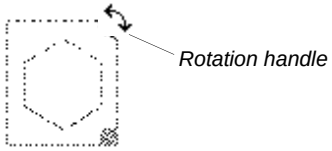
For information about transferring ChemDraw pictures to other types of documents see "Autoscaling" on page 193.

Rotating Objects

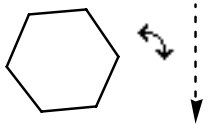
To rotate objects:

1. Select the objects to rotate using a selection tool.

   The Rotation handle is located on the upper right corner of the selection rectangle



2. Drag the Rotation handle clockwise or counterclockwise.



The screen and Info window indicate the magnitude of the rotation around the center of the Selection rectangle.

By default, atom labels do not rotate with the structure.

To rotate an atom label with a structure:

- Press **Ctrl** or **Command** while dragging the structure.

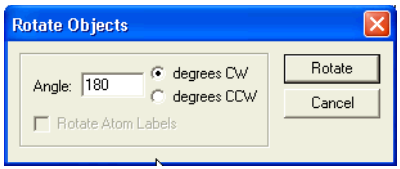
If a single atom is unselected when a structure is rotated, the structure rotates around the unselected atom.

NOTE: *Captions and atom labels that contain multiple colors change to the foreground color when rotated. However, all colors contained in the captions are printed.*

To rotate the selected objects a specified number of degrees:

1. Do one of the following:
   - From the **Object** menu, choose **Rotate**.
   - Double-click the rotation handle.

   The Rotate Objects dialog box appears.



2. Type a number and click **degrees CW** for a clockwise rotation or **degrees CCW** for counterclockwise rotation.
3. If you want to rotate the atom label text, click **Rotate Atom Labels**.
4. Click **Rotate**.

   Objects are rotated around the center of the Selection rectangle.

To repeat the same rotation on any object in the document window:

1. Immediately after performing a rotation, select the other objects to rotate.
2. From the **Edit** menu, choose **Repeat Rotate**.

Structure Perspective

You can rotate molecules or portions of molecules through three dimensions with the Trackball tool . The Trackball behaves similarly to the Marquee tool.

To rotate a structure:

1. Select the structure by dragging over it with the Trackball tool.
2. Place the cursor inside the marked rectangle and drag in any direction.

   The structure will rotate on the X or Y axis, or a combination of X and Y.
3. Use Shift+drag to limit the rotation to the X or Y axes only.

You can also select part of a complex molecule and rotate it around a particular bond.

NOTE: *Do not try to use the Trackball to rotate objects such as orbitals or boxes. It was designed to manipulate chemical structures only.*

Flatten Command

Although the Trackball tool is not intended to be a 3D modeling tool, it does introduce z-coordinate information that is saved in .cdx files. This pseudo-3D structure can be confusing when opening files that have been saved after perspective manipulation.

To remove perspective information:

1. Select a structure with the Marquee or Lasso Tool.
2. On the **Object** menu, click **Flatten**.

   All z-coordinate information is removed from the structure.

Reflecting Objects Through Planes

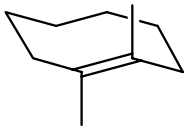
You can reflect structures through planes perpendicular to the X-axis or Y-axis using a selection tool. Used with duplicating, you can create mirror images of chemical structures for representing racemic mixtures and other stereoisomers.

Flipping Objects

To reflect an object through a plane perpendicular to the X-axis:

1. Select the objects to reflect.

2. From the **Object** menu, choose **Flip Horizontal**.



Atom labels and captions do not flip along with the object.

To reflect an object through a plane perpendicular to the Y-axis:

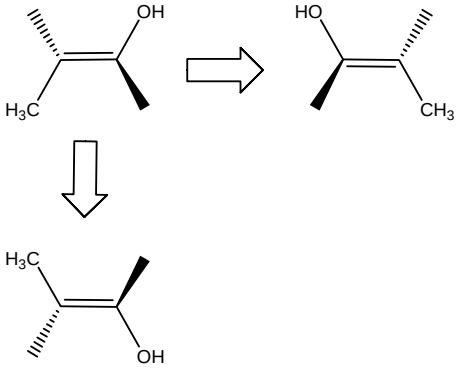
1. Select the objects to reflect.
2. From the **Object** menu, choose **Flip Vertical**.

Creating Mirror Images

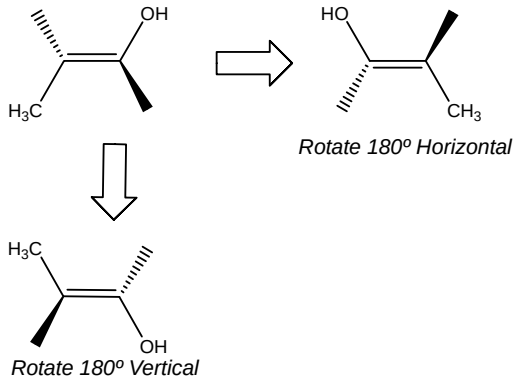
You can create mirror images from structures with defined stereochemistry by duplicating the structure and then rotating it.

To create a mirror image:

1. Draw a structure with defined stereochemistry, for example, wedged bonds.
2. Select the structure and make a copy with **Ctrl+Drag** or **Option+drag**.
3. While the copy of the structure is still selected, choose **Flip Horizontal** or **Flip Vertical** from the **Object** menu.



You can also preserve the absolute stereochemistry while flipping by using the **Rotate 180°** commands on the **Object** menu.



Resizing Objects

You can resize objects by dragging the resize handle of a selected object or by scaling. If all objects in the document window are part of the selection, after

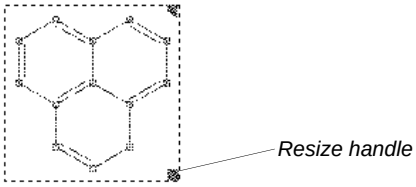
you resize, a message appears asking whether you want to change the document settings for that document. If you do so, all subsequent bonds, atom labels, and captions are drawn using the new settings.

The Resize Handle

To resize an object or collection of objects:

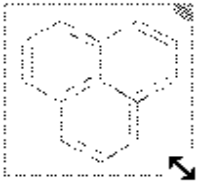
1. Select the objects to resize.

   The resize handle is located in the lower right corner of the selection rectangle.



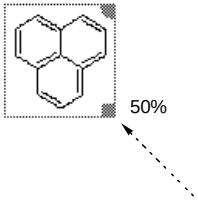
2. Point to the **Resize handle**.

   The cursor becomes a double-headed arrow.



3. Drag the resize handle until the object is the size you want.

   The screen and Info window indicate the percentage enlarged or reduced.

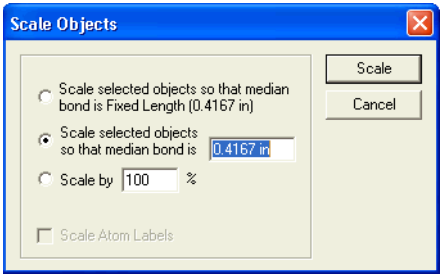


Scaling Objects

To resize objects with the Scale command:

1. Select the objects to scale.
2. Do one of the following:
   - From the **Object** menu, choose **Scale**.
   - Double-click the **Resize handle**.

   The Scale Objects dialog box appears.



Use the first two options in the Scale Objects dialog box to scale all selected objects so that the median selected bond has a specified length based on the following scale factor:

$$\text{scale factor} = \frac{\text{new median bond length}}{\text{current median bond length}}$$

To scale bonds so that the Fixed Length becomes the new median bond length:

1. Select the top option.

   The fixed length presently in the Drawing Settings dialog is shown in parentheses at the end of the line for this button.
2. Click **Scale**.

To scale the bonds to a new fixed length that you specify:

1. Select the middle option.
2. Type the new median bond length in the box to the right of the button.

3. The current median bond length for the selection is shown in the highlighted text box when the dialog box initially appears.
4. Click **Scale**.

To scale objects by a percentage:

1. Click **Scale by**.
2. Type the percentage in the box to the right of the button.
3. Click **Scale**.

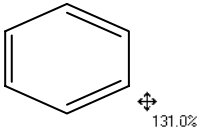
This is the only available option when the selection does not contain any atoms or bonds.

Distorting a Selection

In most cases, when you resize an object, the aspect ratio of the object (the ratio of the height to width) does not change. However, it is possible to change the aspect ratio (distort) of certain objects including chemical structures, circles, boxes, and ovals.

To distort an object in the horizontal or vertical direction:

1. Select the object and **Shift+drag** the Resize handle.



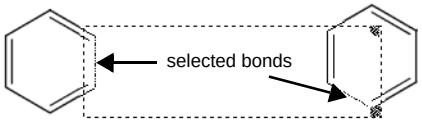
   Shift modifies the resize operation so that you can distort objects along the X-axis or Y-axis.
2. Drag the Resize handle in the desired direction.

Joining Objects

Use the Join command in the Object menu to fuse two chemical structures together. Once structures are joined they can be easily selected by double-clicking.

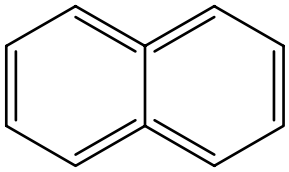
To join chemical structures along the length of a bond:

1. Select a bond or atom in one of the molecules
2. Shift+click to select the corresponding bond or atom on the second molecule that you wish to fuse.



3. From the **Object** menu, choose **Join**.

   The structures are joined.



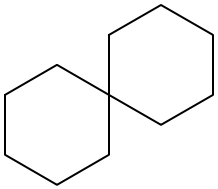
To join chemical structures at one atom to create a spiro linkage:

1. Position the two chemical structures so that the atoms you wish to fuse are more or less opposite each other.

NOTE: While you no longer have to position the chemical structures exactly, attempts to fuse atoms that are not approximately lined up will lead to incorrect results.

2. Select the two atoms to be fused.

3. From the **Object** menu, choose **Join**.



NOTE: *When you join two differently colored bonds or atom labels, the color of the front object becomes the color of the resulting joined object. When you join two atoms that are labeled, the front atom label becomes the atom label of the resulting atom. For more information about front to back ordering of objects, see Chapter 11: "Working With Page Layout".*

Grouping Objects

You can group a number of objects drawn separately. Grouping creates an association between objects so they can be easily selected. You can select all grouped objects by double-clicking with a selection tool. Objects within a group can be selected individually and manipulated while still remaining part of the group.

If you want to group objects so that the individual objects in the group *cannot* be accessed, you can create an Integral group. When you select any object in an Integral group, the entire group is selected.

Grouping does not lock the position or orientation of objects. Grouped objects maintain their relative positions when they are centered on the page, aligned or distributed.

Atoms and bonds making up a single chemical structure are always grouped. If you group part of a structure with other objects, the resulting group contains the entire structure. If you add atoms or bonds to a grouped structure, the new atoms and bonds are part of the group.

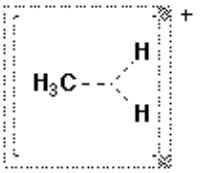
To group several objects:

1. Select the objects to group using a selection tool.
2. From the **Object** menu, choose **Group**.

To select an individual object within a group:

- Move the selection tool over an object until it is highlighted and click once.

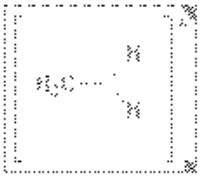
  The object is selected, not the group.



To select grouped objects:

- Move the selection tool over an object until it is highlighted and double click

  The entire group is selected.



Ungrouping Objects

To ungroup objects that are grouped:

1. Select a group, as above.
2. From the **Object** menu, choose **Ungroup**.

   All the objects previously grouped become individual objects.

Creating Integral Groups

To create a group in which individual objects cannot be accessed:

1. Select the objects to group using a selection tool.
2. From the **Object** menu, choose **Group**.

3. With the group selected, right-click, point to **Group**, and then click **Integral**.

To restore an Integral group to a regular group:

1. Select the Integral group.
2. Right-click, point to **Group**, and then deselect **Integral**.

Chapter 8: Advanced Drawing Techniques

Overview

ChemDraw provides advanced drawing features that allow you to:

- Label functional groups with Nicknames.
- Contract and expand sections of structures.
- Add bonds to specific characters in atom labels.
- Create bonds whose attachment is not explicitly defined.
- Color objects.
- Draw with Templates.
- **Pro** Clean up structures.

Using Nicknames

Nicknames allow you to create short names for functional groups to use as an atom label or part of a label. When an atom is labeled with a Nickname, the chemical significance of the expanded structure is retained.

Commonly used Nicknames, such as Me, Et, and Ph are provided with ChemDraw in the **ChemDraw Nicknames** file located in your ChemDraw Items folder. You can edit this list using tools in ChemDraw. You should not attempt to edit this file directly.

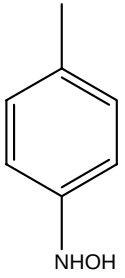
You can assign HotKeys to Nicknames. For example, in the Nicknames and HotKeys provided with ChemDraw, the Hotkey, "4" labels an atom with "Ph" which is a Nickname representing a phenyl group. For more information, see "Labeling Atoms with HotKeys" on page 87.

You can use Generic Nicknames when drawing query structures. For more information, see "Generic Nicknames" on page 161.

Applying Nicknames

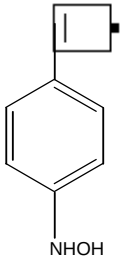
To use a Nickname to label an atom:

1. Create a structure.

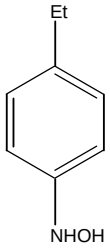


2. Double-click an atom with a bond tool or click an atom with the **Text** tool.

   An atom label text box appears.



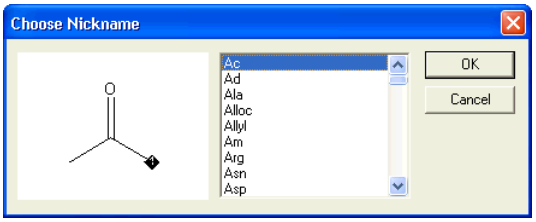
3. Type a Nickname label such as “Et”.



To select a Nickname to apply to an atom using a Hotkey:

1. Point to an atom.
2. Press the Hotkey “=”.

   The Choose Nickname dialog box appears.



3. Select a Nickname from the list.
4. Click **OK**.

NOTE: *Nicknames are tokens and do not flip orientation when applied to the left side of a structure when using Automatic Justification. For example, in the absence of a defined Nickname, the label “OTHP” appears as “PHTO” when applied to the left side of a structure. However, since the Nickname “THP” is defined, the label appears as “THPO”. For more information, see “Aligning Text” on page 81.*

Pro Defining Nicknames

To define your own Nicknames, you must have ChemDraw Pro.

You can define Nicknames with one or two attachment points. The attachment points must be single bonds.

To define a new Nickname:

1. Create a structure containing the functional group you want to define as a Nickname.
2. Select the functional group.

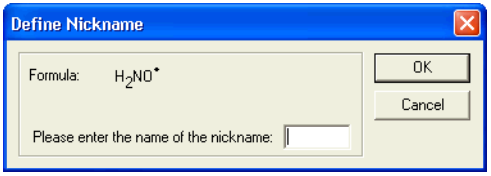
You must indicate the connection point for the functional group by selecting the new fragment without the bond connected to the attachment point.

NOTE: *If stereochemistry is indicated in a structure that you are defining as a Nickname, the stereochemistry is retained.*

---

3. From the **Structure** menu, choose **Define Nickname**.

   The number of connection points is shown by radicals in the Formula. You can have only one or two connection points in a nickname.



4. Type a short name for the Nickname.
5. Click **OK**.

   The Nickname is defined.

If you use a Nickname that is the same as an element name, a message indicates that the element is replaced with the Nickname. For example, using Ac for an acetyl group replaces the element Actinium. The Check Structure command recognizes the label as an acetyl group rather than Actinium.

ChemDraw provides the following default Nickname/Element conflicts:

Symbol	Nickname	Element
Ac	Acetyl	Actinium

Am	Amyl	Americium
Np	*para*-Nitrophenyl	Neptunium
Pr	Propyl	Praeseodymium

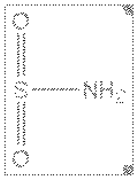
To remove the overriding Nicknames, choose List Nicknames from the File menu and delete the overriding Nickname definition. For more information, see "Deleting Nicknames" on page 124.

Troubleshooting Nicknames

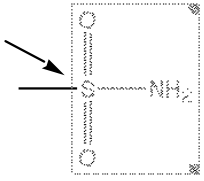
If the command Define Nicknames is dimmed, check for the following:

- A connection point is not present
- More than 2 connection points are defined
- The connection point is not a single bond

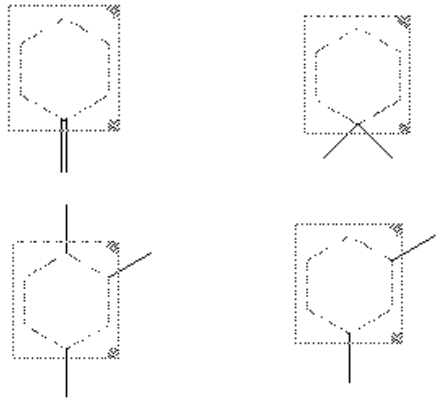
In the example below, the functional group was drawn and the entire group selected. Because there is no atom that indicates a connection point, you cannot define a Nickname.



In the example below, the sulfonamide group is attached to an unselected bond, which defines a bond from sulfur as the connection point for the group. This allows you to define a Nickname.

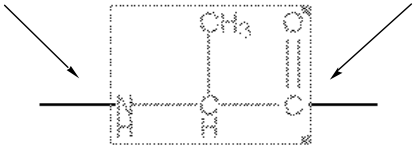


You must leave a bond unselected for each connection point. You cannot define more than two connection points or one attachment point on a single atom in a nickname.



incorrect definitions correct definitions

The definition in the figure below was used for the amino acid, Ala. The unselected bond at each end of the structure indicates the connection points—Nitrogen on the left and Carbon on the right.



You can draw a peptide chain by:

- Stringing Nicknames together.

H——Gly—Ala—OH

- Stringing Nicknames together in an atom label as long as there is a bond attached.

H——GlyAlaOH

- Stringing Nicknames together and not including bonds.

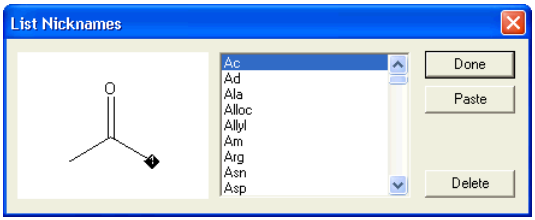
HGlyAlaOH

Viewing Nicknames

To view the list of defined Nicknames:

- From the **File** menu, choose **List Nicknames**.

  The List Nickname dialog box appears.



To insert a nickname into your document:

1. Select the nickname.
2. Click **Insert**.

   The nickname appears in your document.

Deleting Nicknames

To delete a Nickname:

1. From the **File** menu, choose list **Nicknames**.
2. Select the Nickname that you want to delete from the list.
3. Click **Delete**.

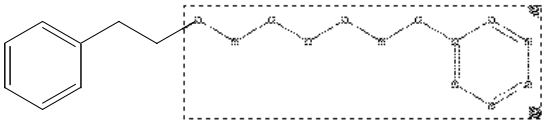
   The Nickname is removed from the list.

Pro Contracting Labels

You can compress an area of a structure and replace it with a text label by using the Contract Label command. Contracted labels are similar to Nicknames, but they are for one-time use only, in the current document.

To create a contracted label:

1. Select the area of the structure to contract.

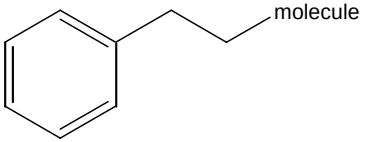


2. From the **Structure** menu, choose **Contract Label**.

   The Contract Label dialog box appears.

3. Type a label for the contracted structure and click **OK**.

   The label replaces the selected portion of the structure.

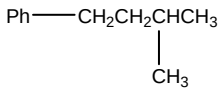


NOTE: *If the area of the structure you contract contains errors, an error dialog box appears. Click Ignore to view any other errors. Click Ignore All to ignore all errors or Stop to end the contract process.*

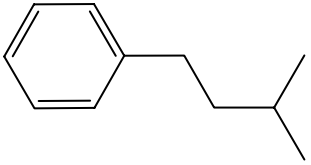
Pro Expanding Labels

If your structures contain defined nicknames, long atom labels, or contracted labels, ChemDraw can restore your structures to the fully expanded form.

Contracted Form



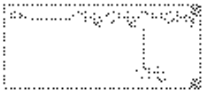
Expanded Form



When you expand a label containing a divalent nickname, for example HAlaOH, the first attachment is to the character left of the nickname (H). The second attachment is to the character right of the nickname (OH).

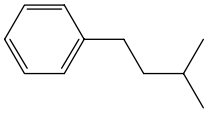
To expand atom labels:

1. Select a selection tool.
2. Select the label to expand or double-click the structure to expand all possible labels.



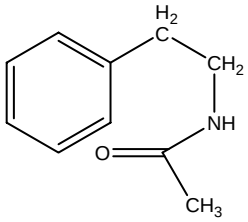
3. From the **Structure** menu, choose **Expand Label**.

   Your structure is redrawn in its expanded form.

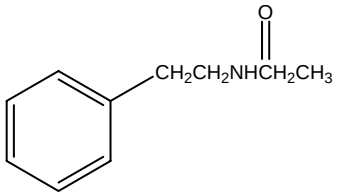


Multi-Attached Labels

Multi-attached atom labels enable you to draw chemical structures more efficiently by allowing you to attach bonds anywhere along an atom label.



Expanded structure



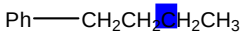
Compact structure with multi-attached atom labels

Adding Bonds to an Atom Label

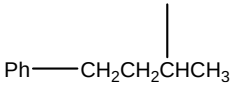
To add bonds to an atom labels:

1. Draw the structure and attach any necessary atom label.
2. Select a **Bond** tool.
3. Position the cursor where you want to attach additional bonds.

   The selected part of the atom label is highlighted.



4. Click and drag from the atom label to draw your bonds.

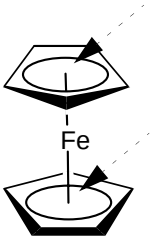


You can determine the orientation of the resulting bond by dragging. If you click to add a bond, there are several preferential orientations for the resulting bond as outlined below.

- Adding from the end of an atom label creates bonds that are preferentially horizontal.
- Adding from the middle of an atom label creates bonds that are preferentially vertical.
- Adding from the start of an atom label creates bonds that try to attain the chain angle setting in the Drawing Settings dialog box. If that angle cannot be attained, the next best angle is used.

Using Multi-Center Bonds

You can draw, with chemical significance, polyhapto structures such as ferrocene ($(Cp)_2Fe$).



Creating a Multi-Center Bond

To create a multi-center attachment point:

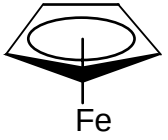
1. Select the structure whose center you want defined as a multi-center attachment point.
2. From the **Structure** menu, choose **Add Multi-Center Attachment**.

   An asterisk is displayed with the fragment to show that it contains a multi-center node.

The asterisk is not visible once a bond is drawn to it. You can view the attachment point with a bond or selection tool. For more information, see "Viewing Attachment Points" on page 127.

To draw a bond to a multi-center attachment point:

1. Click the **Bond** tool.
2. Point to the **asterisk** and either click or drag to create a bond.



To make the bond in ferrocene appear that it is coming from within the ring:

1. Double-click the wedged bond to make it come forward.
2. Select the downward bond.

3. Double-click on the cyclopentadienyl ring with a selection tool.

   The entire structure, including the single bond, is selected. The Cp ring and the single bond are associated as one structural unit because ChemDraw recognizes the bond between them.

NOTE: *For the best looking structure, you may need to draw a longer than normal bond. You can toggle the Fixed Length command by typing* **Ctrl +L** *or* **Command+L**.

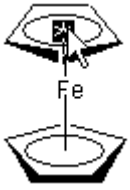
Viewing Attachment Points

After you draw a bond from the multi-center attachment point, the asterisk disappears. You can verify the node is present with a bond or a selection tool. This provides a way to check the definition of a pre-existing multi-center attachment point.

To view a node with a selection tool:

- Select the selection tool and position the cursor over to attachment point.

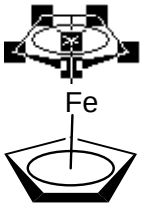
  The attachment node is highlighted.



To view a node with a bond tool:

- Select the bond tool and position the cursor over the attachment point.

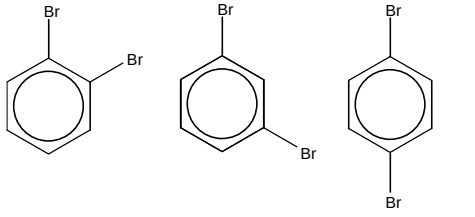
  The attachment node and all the atoms it represents are highlighted.



Pro Using Variable Attachment Positions

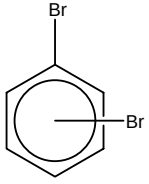
You can use the Add Variable Attachment command to draw different positional isomers of a compound using an abbreviated notation that retains chemical significance.

For example, you can explicitly draw the three isomers of dibromobenzene shown below.



o-Dibromobenzene *m*-Dibromobenzene *p*-Dibromobenzene

Alternately, you can express all three isomers as a single parent structure by using a variable attachment.



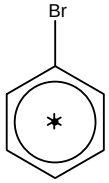
To use variable attachment:

1. Draw the structural fragment to which you want to assign a variable attachment node.
2. Select the fragment using a selection tool.

   TIP: To get the attachment in the center of the ring, select just the ring, not the entire molecule.

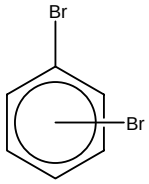
3. From the **Structure** menu, choose **Add Variable Attachment**.

   An asterisk appears in the center of your fragment.



You can treat this attachment node as you would treat the end of a normal bond.

1. Click a **Bond tool**.
2. Point to the asterisk and drag to draw a bond.



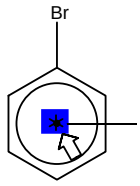
NOTE: *In the example above, Fixed Lengths was disabled using Ctrl+L, or Command+L so a bond could be drawn extending further from the ring.*

After you draw a bond from the attachment node, the asterisk disappears.

To verify that the node is present, do one of the following:

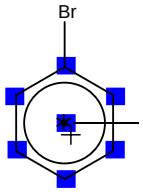
- Click a Selection tool and place the pointer on the attachment point.

  The attachment node is highlighted.



- Click a **Bond tool** and place the pointer on the attachment point.

  The attachment node and the atoms it represents are highlighted.



For more information about viewing the attachment points, see "Viewing Attachment Points" on page 127.

Pro Using Structure CleanUp

The Structure CleanUp command is used to neaten the appearance of molecules by regularizing bond lengths and angles. Graphic objects such as arrows and aromatic circles are not affected. Use Structure CleanUp to redraw structures that you may have drawn freehand or to neaten structures that you may have imported from another application.

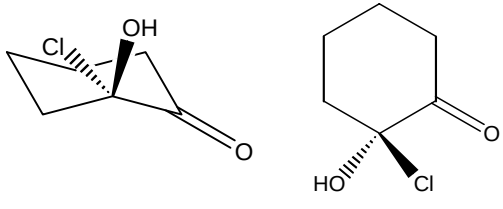
Structure CleanUp may not create *the* best structure. Most structures have many "clean" forms, a problem that is particularly noticeable with straight-chain alkanes.

If you select only part of a structure when you choose Structure CleanUp, the other atoms and bonds are not be affected.

NOTE: *For some compounds, the Structure CleanUp command produces a structure that extends beyond the bounds of the page. To view the entire structure, scale the structure or increase the size of the printed page. For more information, see "Resizing Objects" on page 115 and "Setting up Pages" on page 177.*

General Rules for Structure CleanUp are:

- The Fixed Length setting in the Drawing Settings dialog determines optimum bond lengths.
- A given ring is redrawn only if all of its bonds are selected.
- Multi-attached atom labels and variable attachment points cannot be cleaned.
- Multi-center bonds cannot be cleaned.
- Structures are rotated so that as many bonds as possible are directed at a multiple of 15 degrees.
- Structure CleanUp preserves stereochemical meaning rather than the precise identity of any wedged or hashed bonds, as shown below.

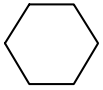


Before *After*

Using Structure CleanUp:

1. Select the structure or part of the structure you want to clean up with a selection tool.

2. From the **Structure** menu, choose **Structure CleanUp**.



NOTE: *Structure CleanUp does not position molecules relative to other objects. Overlap may occur.*

Working with Color

With the color capabilities of ChemDraw, you can create full color presentations of your chemical drawings to appear on your monitor, print on a color printer, or create 35mm slides using a film printer.

Most computers can display any of 16 million colors, but the number of colors that can appear at any one time may be limited by the particular monitor and display card installed in your computer.

In ChemDraw, you can choose from a palette consisting of a Background Color, a Foreground Color, and up to twenty additional colors for any given drawing. A palette is stored in every document and Style Sheet or Stationery Pad. You can use Style Sheets or Stationery Pads to create a series of documents with the same color scheme.

Using color you can:

- Color atoms and bonds in a mostly black-on-white drawing to highlight areas of interest.

- Color parts of a structure in a reaction scheme to indicate where starting materials end up in the products of a complicated mechanism.
- Use colored boxes and circles to highlight atoms or molecules.
- Create slides that are easier to view by using light objects on a dark background.

Coloring Objects

Any object that you can select with a selection tool can be colored. You can color individual bonds, part or all of a chemical structure, or objects such as boxes, curves, arrows, orbitals and reaction mechanism symbols.

The border of objects that are shaded or filled, such as white filled s-orbitals in the Orbitals palette, are the same color as the shading or fill. The border of objects that are hollow, such as circles and hollow boxes in the Drawing Elements palette can be colored, but the inside of the object cannot.

To color an object:

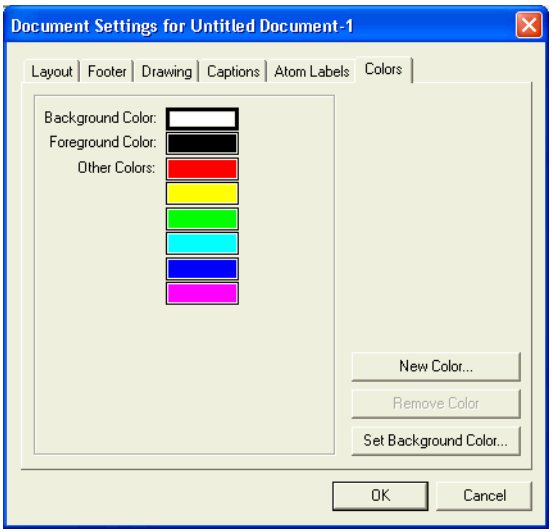
1. Select the object in a document window with a selection tool.
2. Do one of the following:
   - On the **Style** toolbar, click the **Color** button, and select the color from the menu that appears.
   - From the **Color** menu, choose a color.
   - In the **Object Settings** dialog box, on the **Drawing** tab, click the **Color** button , and select the color from the menu that appears.

Displaying the Color Palette

You can use the color palette to specify the color of objects and text in the document within the active window.

To view the Color palette:

1. From the **File** menu, choose **Document Settings**.
2. Click the **Colors** tab.



Use the Color tab to specify the following colors:

- **Background Color**—Fills the background of the current document in the active window.
- **Foreground Color**—Default color used when you draw a new object.
- **Other Colors**—Colors available in the Color Menu for changing the color of individual objects. The colors are represented in the same order that they appear in the Color menu.

You can customize the Color menu. Colors can be added, or existing colors can be changed. Changing a color, for example Other #2, changes all objects that are using the color.

NOTE: *If you select an individual or grouped object that contains multiple colors, there is a check mark next to each of the colors in the Color menu. The purpose of the check marks is to alert you that a change would affect more than one color.*

Customizing the Color Palette

You can add, remove, or change the default foreground and background color and specify the other colors available for coloring objects.

Changes made to the color palette affect the current document only. You can save Color Palette settings (foreground, background, and up to 20 other colors) in a Style Sheet or Stationery Pad. For more information, see "Saving Customized Settings as Style Sheets or Stationery Pads" on page 21.

A summary of each of the options is described in the following table.

Option	Description
New Color	Add a new color box and set its color using the Color Picker or Color Wheel dialog box.
Remove Color	Delete a color box that you have selected in the left side of the dialog box. Any objects using the removed color are changed to the Foreground color.
Set Color	Change the color associated with a color box that you have selected in the left side of the dialog box. Any objects using the old color are changed to the new color.

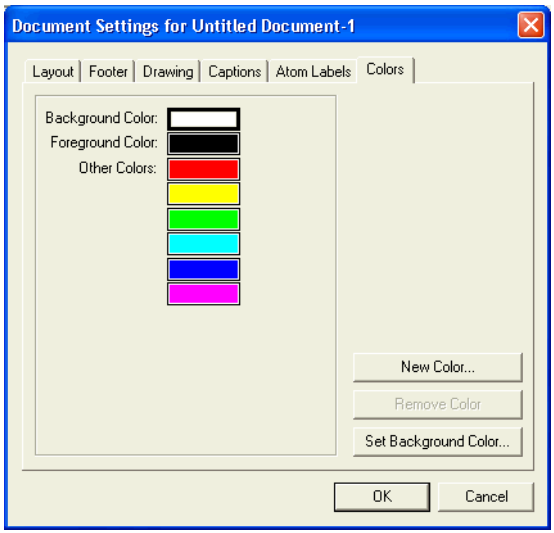
Windows Color Settings

To change the palette of colors used in the current document:

1. From the **File** menu, choose **Document Settings**.

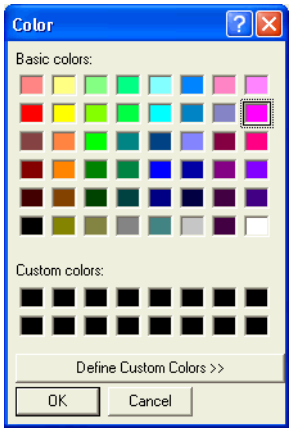
   The Document Settings dialog box appears.

2. Click the **Colors** tab.



3. Double-click the color to change.

   The Color dialog box appears.



4. Click a color box in the Basic Colors or the Custom Colors section.

   A highlighted border appears around the color you select.

5. Click **OK**.

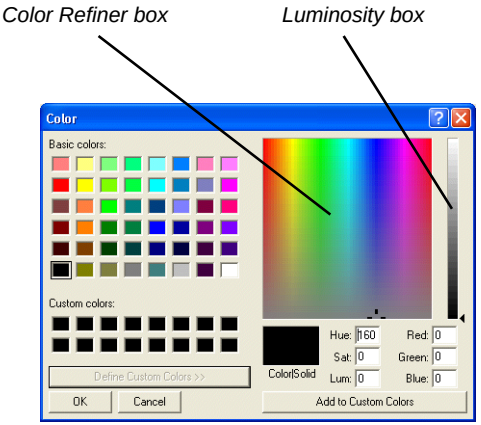
   The color is changed to the new color and added to the Color menu.

Adding or Customizing Windows Colors

To add colors or create customized colors:

1. In the Color dialog box, click **Define Custom Colors**.

   The Color dialog box appears.



2. Click a color in the Color Refiner box to set the hue and saturation.

   The pointer turns into a Crosshair when you click. You can drag to a different region to change the hue and saturation.

3. Click in the Luminosity box to set the brightness of the color.
4. If necessary, change the hue, saturation, luminosity, and RGB components by typing the values in the text boxes.
5. Click **Add to Custom Colors**.

Macintosh Color Settings

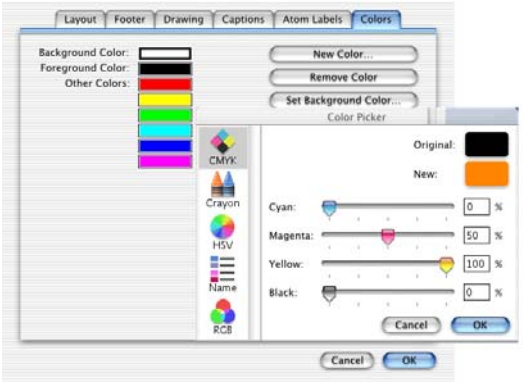
To change the palette of colors used in the current document:

1. From the **File** menu, choose **Document Settings**.

   The Document Settings dialog box appears.

2. Click the **Colors** tab.
3. Click **New Color**.

   The Color Picker dialog box appears.



4. Use one of the icons on the left to select a method of defining your color, then select a color.

   For more information about the Macintosh color options, refer to your System documentation.

5. Click **OK**.

   The new color appears in the Colors tab in place of the original color and is added to the color menu.

Adding or Customizing Macintosh Colors

To add a new color to the Color menu:

1. On the Color tab, click **New Color** or **Set Other Color**.

   The Color Picker dialog box appears.

2. Click a color in the Color Wheel.
3. If necessary, adjust the hue, saturation, brightness, and RGB components by typing the values in
4. Click **OK**.

   The new color is added to the list of Other Colors.

Removing Colors

To remove a color from the Color menu:

1. Click the color you want to remove.

   A highlight box appears around the color.
2. Click **Remove Color**.

   The color disappears from the list of other colors. Objects that were drawn in the removed color are changed to the Foreground color

Templates and Color

The background and foreground colors used in a template from the template pop-up palette are not used when the template is drawn in a document window. However, any other colors used in the template are added to the color palette of the current document if they are not already present. This is part of the autoscale feature. For more information, see "Autoscaling" on page 193.

Saving Color Palette Settings

You can save the Color Palette in a Style Sheet or Stationery Pad. The Color Palette is saved in addition to other document settings such as Page Setup settings, Text settings, and Drawing settings.

Drawing With Templates

Template documents are collections of structures organized by structural type or functionality. A structure in a Template document is named a template. Use an existing template instead of drawing the structure to shorten the time required to create documents.

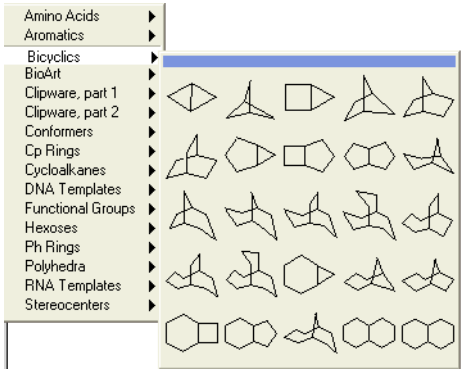
The Template documents distributed with ChemDraw are stored in the ChemDraw Items folder in the same folder as the ChemDraw application.

NOTE: **Pro** *In ChemDraw Pro, you can define your own commonly used structures as templates. Any Template documents in the ChemDraw Folder are listed in the Windows menu (Macintosh) or Open Special on the File menu (Windows).*

The Templates Tool

The Templates tool contains a palette from which you can select different types of structures or objects. The Templates tool has two levels:

- The first level displays the available Template documents.
- The second level displays the templates within each Template document.



NOTE: **Pro** *In ChemDraw Pro the pop-up menu is segmented if any Template documents are open for editing. The upper segment contains Template documents that are currently open for editing.*

Choosing a Template

To choose a template from the Template palette:

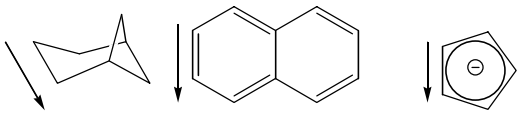
1. Hold down the mouse button over the **Templates** tool .
   A menu listing the Template documents appears.
2. Point to a Template document name.
   A palette containing the available templates appears.
3. Choose a template from the palette.

When you display the Template palette that was last used, a blinking box appears around the currently selected template until you drag to another template.

Using Templates

When you draw with templates, the first bond drawn determines the position of the template in a document window. All remaining bonds are drawn counterclockwise. The most nearly vertical bond on the far-left atom is drawn first, from top to bottom. If there are two equivalent bonds, the atoms that are at a lower position are used to draw the first bond.

Drawing direction of template structures



Templates are automatically scaled to the document settings of the current document in the active window. For more information, see "Autoscaling" on page 193.

After a template is drawn in a document window, the structures or objects can be manipulated by standard drawing and editing methods.

Drawing a Template

To draw a template:

- Click in a document window.
  The template is drawn centered around the pointer in the orientation that it appears in the Templates palette.

Fusing a Template With an Existing Structure

To draw a template and fuse it with an existing structure:

- Click an existing bond in a document window.

To deposit a template and create a spiro-linkage with an existing structure:

- Click an existing atom in a document window.

To draw a template in a document window and control the size and orientation:

- Drag from the beginning of the first bond in the template to the end of the first bond.
  When you drag upwards the bulk of the template is drawn to the left, and when you drag downwards the bulk of the template is drawn to the right. Templates must contain at least one bond in order to be drawn by the dragging method.

Drawing with the Same Template

To draw another template of the same type:

1. Click the **Templates** tool .
2. Draw the template in a document window.

Pro Creating Templates and Template Documents

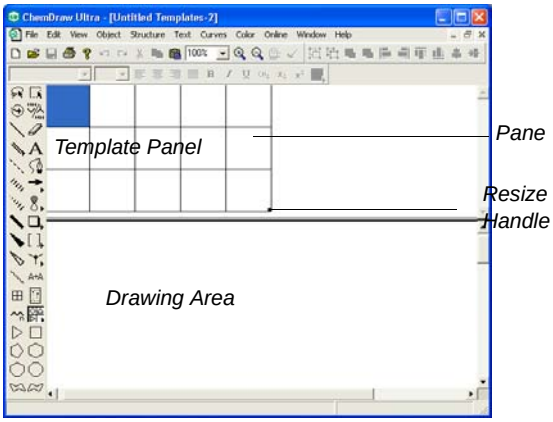
In ChemDraw Pro you can create new templates and add them to existing Template documents or create new Template documents.

To create a new Template document:

- On the **File** menu, point to **Open Special**, and then choose **New Templates**.

A new and untitled Template window appears. The Template window is similar to a document window. The Template window is divided into two halves by a moveable, horizontal line:

- **Template panel**—Top half of the window consists of individual panes where newly created templates appear.
- **Drawing area**—Bottom half of the window where you can draw new templates.



The templates you define are not limited to atoms and bonds. Templates can contain any ChemDraw objects such as captions, boxes, arcs, orbitals, arrows, reaction mechanism symbols, and curves. The ChemDraw objects in Template documents can be colored. However, the colors do not appear in the Templates tool palette. You can paste pictures from other applications into a Template pane. Pasted objects are scaled to the current Template document settings. For more information, see "Autoscaling" on page 193.

Creating Templates

To create a new template:

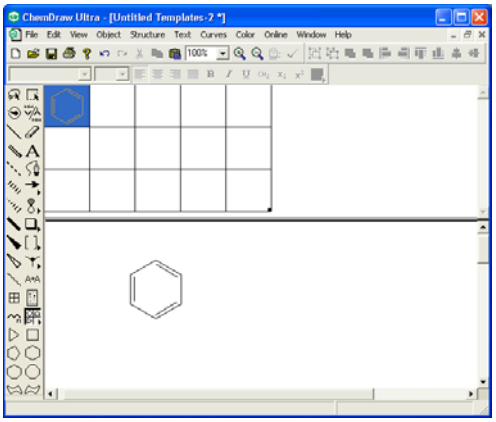
1. Select a Template pane by clicking it.
2. Draw a structure or object in the drawing area of the Template window.

   The structure appears in the Template pane as you draw. The tools in the Tools palette are used to draw a template in the drawing area of the Template window exactly as they are used to draw structures in the drawing area of a document window.

To select a different Template pane:

- Click another Template pane.

  When you select a Template pane, the contents of the pane appear in the drawing area.



As you define templates they become available for use in your document without having to save the Template document.

To view the newly-defined Template:

- Point at the **Templates** tool and hold down the mouse button.

  The name of the new Template document appears in the menu.

Orientation of Templates

To make the templates that you create as easy to draw with as possible, it is recommended that you orient your structures so that the bond that establishes the position of the template, for

example, the bond used for fusing is left and vertical. The most vertical left bond is drawn first. For examples, see "Using Templates" on page 134.

Resizing Template Panes

To resize the Template panes in the Template panel:

- Drag the **Resize handle** on the lower right corner of the Template panel.

  The percentage the block of Template panes is enlarged or reduced appears in the Info window.

Template Panels

To increase the size of the Template panel:

- Drag the Template dividing line.

To add a row of panes to the Template panel:

1. Select a Template pane.
2. From the **Edit** menu, choose **Add Row Before** or **Add Row After**.

   The new row is added before or after the Template pane you selected.

To add a column to the Template panel:

1. Select a Template pane.
2. From the **Edit** menu, choose **Add Column Before** or **Add Column After**.

   The new column is added to the right or left of the Template pane you selected.

To delete a row of Template panes from the Template panel:

1. Select a Template pane in the row you want to delete.
2. From the **Edit** menu, choose **Delete Row**.

To delete a column of Template panes from the Template panel:

1. Select a Template pane in the column you want to delete.
2. From the **Edit** menu, choose **Delete Column**.

   The column is removed and all other columns are moved to the left.

Saving Template Documents

To save a Template document and have it available in the Template pop-up menu and the Window menu:

1. From the **File** menu, choose **Save As**.

   The Save As dialog box appears.

   Saving a Template document in the ChemDraw Items folder makes it accessible in the Open Special submenu and in the Templates tools palette.
2. Type a name for the Template document and click **OK** or **Save**.

Chapter 9: Working With Structures

Overview

You can perform the following functions on the structures you create:

- Check a structure to identify valence and label errors.
- View analysis information about a structure.
- Assign Atom-to-Atom mapping.
- Show Stereochemistry.
- In ChemDraw Pro, display the chemical properties for a structure.
- In ChemDraw Pro, break existing structures across one or more bonds to mimic the fragmentation in a mass spectrometer.
- In ChemDraw Ultra, assign structures to spectra and calculate NMR shift information.

Checking Chemistry

The Check Structure command identifies valence and label errors in your structure.

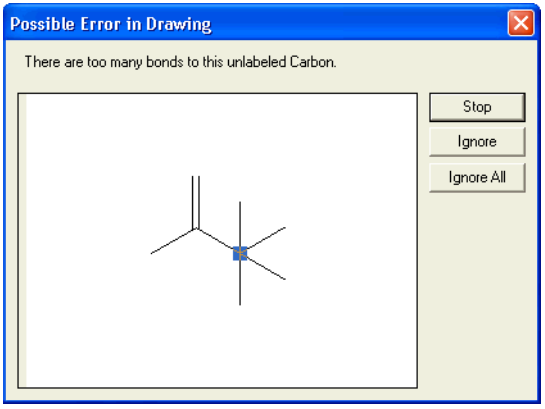
Check Structure

You can check the chemistry of a selected structure, part of a structure, or caption (in Formula style) with the Check Structure command. The structure is checked using normal valences and elements, and defined Nicknames.

To check the valences of all selected atoms in a structure:

1. Select a structure, part of a structure, or caption with a selection tool.
2. From the **Structure** menu, choose **Check Structure**.

   Each label in the structure is checked. sequentially. When a label is incorrect, a message window appears.



To continue checking the structure when a message appears:

- Click **Ignore**.

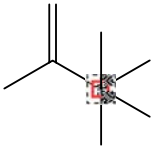
To ignore all subsequent errors in a structure:

- Click **Ignore All**.

To stop checking a structure when a message appears:

- Click **Stop**.

The check ends and the atom that is causing the problem is selected.



Check Structure when Copying to Clipboard or Exporting

To have ChemDraw perform a check structure analysis on any structure copied to the Clipboard:

1. From the **File** menu, choose **Preferences**.
2. Click the **Check Structure When Copying to Clipboard or Exporting** check box.

This change affects all documents.

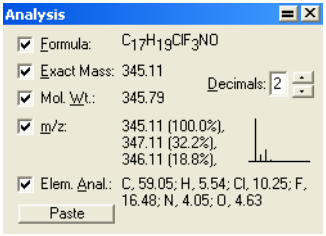
Viewing Analysis Information

The Analysis window displays the chemical formula, exact mass, molecular weight, m/z, and elemental analysis for the entire document, a structure, part of a structure, or a caption in Formula style.

To view analysis information:

- From the **View** menu, choose **Show Analysis Window**.

  The Analysis window appears.


Analysis
Formula: $C_{17}H_{19}ClF_3NO$
Exact Mass: 345.11
Mol. Wt.: 345.79
Decimals: 2
m/z: 345.11 (100.0%), 347.11 (32.2%), 346.11 (18.8%),
Elem. Anal.: C, 59.05; H, 5.54; Cl, 10.25; F, 16.48; N, 4.05; O, 4.63
Paste

Values for selected objects in the document window are shown. If nothing is selected in your document, values for the entire document are shown.

You can have this window open as you draw in the document. It shows the current values as you draw.

The Decimals setting applies to Exact Mass, Molecular Weight, and m/z only.

The following table describes the analysis properties.

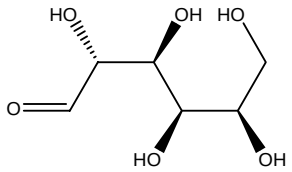
Property	Description
Formula	The molecular formula showing the exact number of atoms of each element in the molecule and charges, radicals, and isotopes.
Exact Mass	The exact molecular mass of the structure, where atomic masses of each atom are based on the most common isotope for the element.
Molecular Weight	The average molecular mass of the structure, where atomic masses are based on the natural abundance of all isotopes of the element.

Property	Description
m/z	Mass/charge, where charge =1. The weights of the most common isotopes and a graphical representation of the isotopic abundance is shown. The molecular weight shown takes the isotopes for each atom and their natural abundance into account. Where there is more than one abundant isotope, ChemDraw computes multiple molecular weights. Low abundance combinations (whether because the isotope is in low abundance or because it includes many moderate-abundance contributions) are not taken into account. *NOTE: You cannot paste the graph in a document.*
Elemental Analysis	The percent by weight of each element in the structure.

To paste information about a structure as a caption:

1. Click the check boxes for the information that you want to paste.
2. Click **Paste**.

The information appears as a multiline caption below the structure. You can edit this information with the text tool.

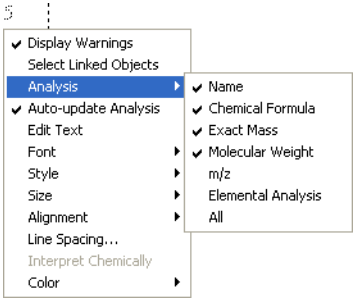


glucose

Chemical Formula: $C_6H_{12}O_6$
Exact Mass: 180.06
Molecular Weight: 180.16
m/z: 180.06 (100.0%), 181.07 (6.9%), 182.07 (1.4%)
Elemental Analysis: C, 40.00; H, 6.71; O, 53.29

The information in the label updates automatically as you edit the structure. You can show or hide the information as follows:

1. Right-click in the label. It does not matter which tool you are using.
2. Point to **Analysis**, and select or deselect the item you want to show/hide.



Showing Stereochemistry

When the Show Stereochemistry option is selected, ChemDraw calculates the absolute stereochemistry for tetrahedral atoms and double bonds according to the Cahn-Ingold-Prelog (CIP) priority rules. For more information about the CIP rules, see "Stereochemistry" on page 236.

Only tetrahedral and double-bond stereochemistry are supported, and only non-racemic stereochemistry is interpreted. Stereochemical indicators for aromatic bonds are not shown.

ChemDraw calculates and displays the following stereochemical terms:

- **(R), (S)**—Standard tetrahedral stereochemistry
- **(r), (s)**—Tetrahedral stereochemistry determined by other stereochemical centers. For example: *cis*-decalin and *myo*-inositol.
- **(E), (Z)**—Standard double-bond stereochemistry

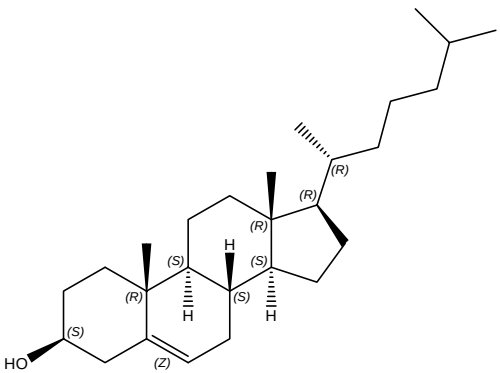
The atom label settings determine the font style and size of the terms.

Stereochemistry Indicators

To show the stereochemistry of a structure:

- Select a structure, right-click, and then click **Show Stereochemistry**.

  The stereocenters are marked as shown in the following example.



cholesterol

If you make changes to the drawing that affect the stereochemistry, the stereochemistry is recalculated.

Hiding Indicators

To hide an individual indicator:

1. Select the indicator to hide.
2. Right-click and choose **Hide Indicator**.

Removing Indicators

To delete an indicator:

1. Click the indicator.
2. Click the eraser tool and then click the indicator.

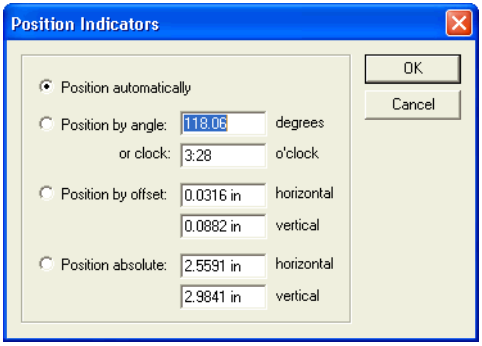
Positioning Indicators

Stereochemistry indicators are positioned automatically and move appropriately if a structure is modified. You can reposition them by dragging them to the desired position or with the Indicator Position dialog box.

To reposition an indicator numerically:

1. With a selection tool, click the indicator to move.
2. Right-click and choose **Position**.

   The Position Indicator dialog box appears.



3. Click the appropriate Position option, and type a value:

To Position ...	Type a value for the position by...
from the atom or bond center to indicator center	angle, in degrees or clock, in clock time
from the atom or bond center to bottom left of indicator baseline	offset, horizontal and vertical
at specified coordinates	absolute, horizontal and vertical

Converting Structures to 3D

You can convert a two-dimensional structure drawn in ChemDraw to a three-dimensional structure. To use this feature, you must have CambridgeSoft Chem3D installed on your computer.

To convert a structure to 3D:

1. Select the structure to convert.
2. From the **Edit** menu, choose **Get 3D Model**.

   The 3D structure appears in the document window.

NOTE: *3D Objects inserted in this way cannot be transferred between platforms. For more information see* *"File Formats" on page 197*.

To edit the 3D structure:

1. Double-click the 3D structure.

   Chem3D opens.
2. Edit the structure and close Chem3D when you are finished.

   The edited structure appears in the ChemDraw document window.

Pro Viewing Chemical Properties

ChemDraw Ultra, using an add-on, ChemProp, calculates predicted values for the physical and thermodynamic properties of a selected structure of up to 100 atoms. You can view the values in the Chemical Properties window.

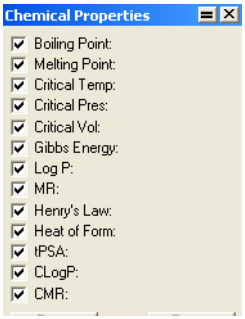
The properties are calculated using the most reliable methods for calculation for the given structure. Log P and MR values based on literature values rather than a calculation are included in the report file.

Viewing the Chemical Properties Window

To view predicted properties for a selected structure:

1. Select the structure to analyze.
2. From the **View** menu, choose **Show Chemical Properties Window**.

   The Chemical Properties window appears.



The following basic values are displayed.

Property	Description
Boiling Point	The boiling point for the structure. Reported in Kelvin at 1 atm.
Melting Point	The melting point for the structure. Reported in Kelvin at 1 atm.
Critical Temperature	The temperature above which the gas form of the structure cannot be liquefied, no matter the applied pressure (T_c). Reported in Kelvin.
Critical Pressure	The minimum pressure that must be applied to liquefy the structure at the critical temperature (P_c). Reported in bars.
Critical Volume	The volume occupied at the compound's critical temperature and pressure (V_c). Reported in cm^3/mol.
Gibbs Energy	The Gibbs free energy, ΔG, for the structure. Reported in kJ/mol at 1 atm and 298.15K.
Henry's Law	The inverse of the logarithm of Henry's law constant [-log (H)] (no units).
Heat of Formation	The heat of formation, ΔH_f, for the structure. Reported in kJ/mol at 1 atm and 298.15K.
tPSA	Calculation of polar surface area based on fragment contributions.
CLogP **Ultra**	The calculated *n*-octanol/water partition coefficient (log P_{ow}).
CMR **Ultra**	The calculated Molar Refractivity

NOTE: *The CLogP and CMR algorithms incorporated in ChemDraw are licensed from BioByte Corp, and have been extensively tested and peer-reviewed as providing highly accurate results. The values produced by these algorithms in ChemDraw should be exactly the same as values produced by the standalone CLogP and CMR applications from BioByte.*
For further information about CLogP and CMR, please refer to the BioByte web site at:
http://www.biobyte.com
and to the manuals for ClogP and CMR at:
http://clogp.pomona.edu/medchem/chem/papers/14-clogp.html
and
http://clogp.pomona.edu/medchem/chem/papers/13-cmr.html

To paste the basic properties into your document:

- Click **Paste**.

To create a report and view results for other fragmentation methods including the Broto, Crippen, Viswanadhan, Joback, and Joback/Stein methods:

- Click **Report**.

When you create a report, a detailed list of information used for performing the calculation is shown in a text file. The list includes additional properties and literature references used to perform the calculation.

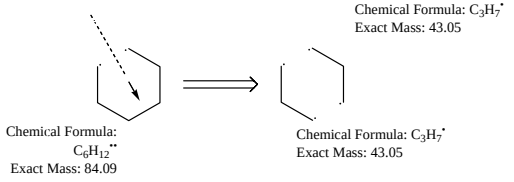
Pro Mass Fragmentation Tool

The Mass Fragmentation tool allows you to break existing structures across one or more bonds. This mimics the molecular fragmentation in a mass spectrometer, but does not have any predictive qualities: you must specify what bonds are to be broken.

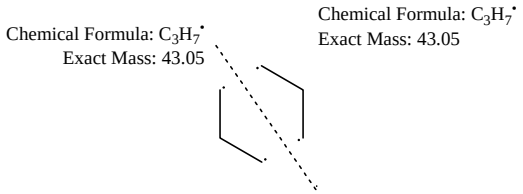
To fragment a structure:

- Drag the mouse across one or more bonds.

  A line is drawn across the bonds that disappears when you release the mouse button. The operation is not final until the mouse is released. This means you can drag the line around holding the mouse button down to see different possibilities, and still back out without breaking any bonds. When the mouse button is released, any bonds crossed by the line are broken

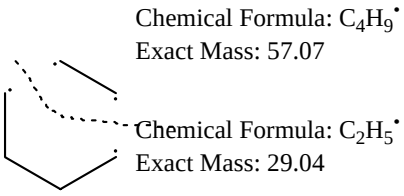


If you want the line to remain on display, hold down the **Alt** or **Option** key after drawing the line.



NOTE: *The order in which you release the mouse button and the Alt or Option key determines whether the line remains displayed or not. Releasing the mouse button first leaves the line displayed.*

The **Alt** or **Option** key also allows you to "turn corners" and cut more than one bond.



When the line crosses a bond, the formula and exact mass for the fragments on either side of the bond are displayed as if the bond were homolytically broken. That is, a single bond turns into a monoradical on each fragment; a double bonds turns into a pair of diradicals. If more than one bond is crossed, all fragments on each side of the line are considered together. If the only bond crossed is a ring bond, a single formula/mass pair is displayed.

NOTE: *It is possible to draw lines that tie themselves in knots. Use this tool with caution to avoid unrealistic fragmentation.*

You can reposition the formula and mass displays (they are text objects), or delete them altogether.

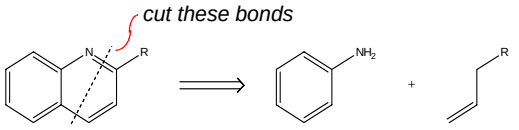
Mass Fragmentation tool procedures:

operation	behavior
drag	Breaks bond(s). The action does not take place until you release the mouse button, so you can "test alternatives".
drag, holding down the Alt or Option key	Draws a freehand line. If you release the mouse button before releasing the Alt or Option key, the dashed line display remains.
drag across a bond, then press the Alt or Option key.	Allows you to change direction and draw a polyline. If you release the mouse button before releasing the Alt or Option key, the dashed line display remains.

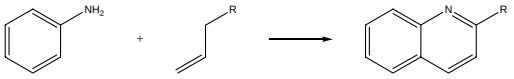
Pro Drawing Reactions

Two new tools speed the drawing of synthesis reactions. Both tools are used in a similar manner to the Mass Fragmentation tool: they are used to cut a bond or bonds in a product. The Dissociation tool draws the resulting fragments as a standard reaction. The Retrosynthesis tool draws the reaction with the product on the left and a broad arrow pointing to the reactants, as is customary in retrosynthetic analyses. In most cases, you will have to clean up the reaction by adding or deleting atoms or bonds.

The following example cuts two bonds, and gives the results shown:

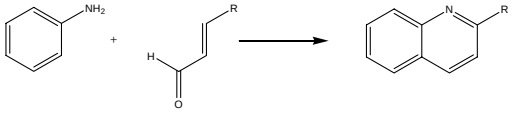


Reaction created with the Retrosynthesis tool



Reaction created with the Dissociation tool

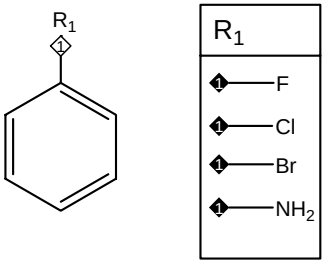
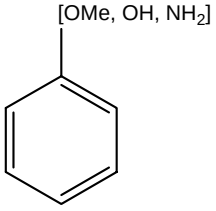
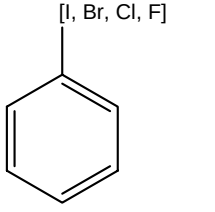
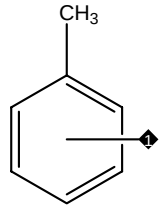
The result is a reasonable approximation of the Beyer Method for quinolines, and can quickly be cleaned up to the correct reaction:



These tools are found in the Fragmentation tools section of the Main tools palette.

Pro Expand Generic Structures

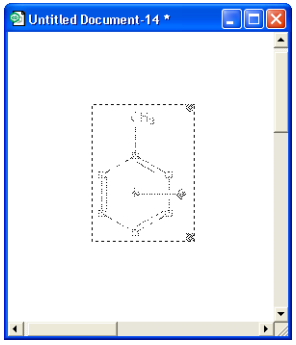
You can generate multiple structures from an abbreviated combinatorial structure with ChemDraw's **Expand Labels** tool . The tool is designed for "small" expansions, and is limited to a maximum of 500 generated structures. For large combinatorial expansions, use CambridgeSoft's *CombiChem for Excel*. Four kinds of abbreviated combinatorial definitions may be used:

definition	example
Alternative Groups and R-tables	
Anonymous Alternative Groups	
Element Lists	
Variable Attachment	

Definitions are expanded into multiple complete molecules. If more than one site is present in the selection, the expansion will include all permutations of substitutions. Expansions are generated into a new document.

To generate a combinatorial library:

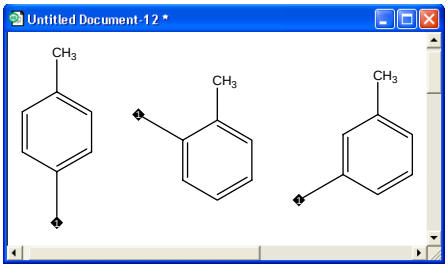
1. Select at least one combinatorial substitution definition.



> ***NOTE:*** *For alternative group/R-tables, both the alternative group label and the table must be selected. If the label is selected but not the table, the label will not be modified by the expansion, and will appear as a label in all generated structures.*

2. Choose **Expand Generic Structure** from the **Structure** menu.

The structures are generated to a new document.



Ultra Spectrum-Structure Assignments

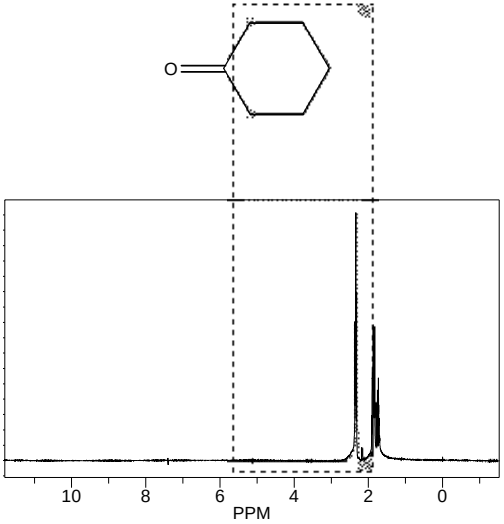
ChemDraw Ultra enables you to assign structures to spectra.You can then display the structure associated with a specific peak by placing the pointer on that peak.

Assigning Structures to Spectra

To assign structures to a spectrum:

1. Open a spectral file.
2. Draw the structure or structures you want to assign to the spectrum.
3. Select specific atoms and bonds in the structure.
4. Shift-click the peak or peaks to which you want the structure assigned.

The selection rectangle surrounds the selected objects.



5. From the **Structure** menu, choose **Make Spectrum-Structure Assignment**.

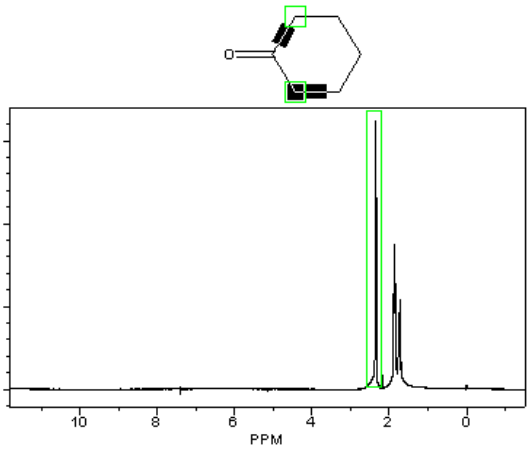
   The selected atoms and bonds in the structure are associated with the selected spectral peaks.

Viewing Spectral Assignments

To view the spectral assignments:

1. Click the Lasso or Marquee tool.
2. Place the pointer over a peak.

The assigned atoms or bonds are highlighted.



Removing Spectral Assignments

To remove spectrum to structure assignments:

1. Click the Lasso or Marquee tool.
2. Select the objects from which to remove the assignment.
3. From the **Structure** menu, choose **Clear Spectrum-Structure Assignment**.

Ultra NMR Shift Information—ChemNMR

ChemNMR is a feature of ChemDraw Ultra only. ChemNMR estimates and displays proton and carbon-13 chemical shifts in ppm for a selected molecule.

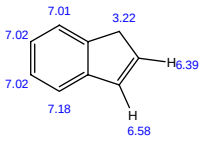
To view ^{1}H or ^{13}C NMR information:

1. Select the target chemical structure.

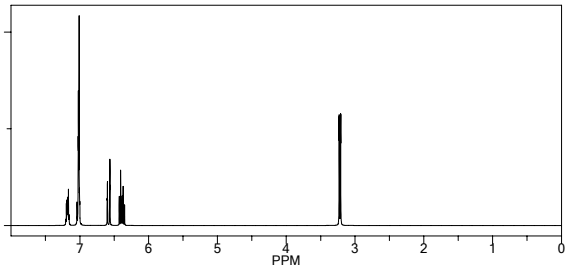
2. From the **Structure** menu, choose **1H-NMR Shifts** or **13C-NMR Shifts**.

   ChemNMR redraws the molecule with the estimated shifts and displays the information and line spectrum in a new window as shown below.

ChemNMR H-1 Estimation



Estimation Quality: blue = good, magenta = medium, red = rough



Protocol of the H-1 NMR Prediction:

Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
CH	7.02	7.26	1-benzene
		-0.12	1 -C=C
		-0.12	1 -C
CH	7.02	7.26	1-benzene
		-0.05	1 -C=C
		-0.19	1 -C
CH	7.18	7.26	1-benzene
		0.04	1 -C=C
		-0.12	1 -C
CH	7.01	7.26	1-benzene
		-0.05	1 -C=C
		-0.20	1 -C
CH2	3.22	1.37	methylene
		1.22	1 alpha -1:C*C*C*C*C*C*1
		0.63	1 alpha -C=C
H	6.58	5.25	1-ethylene
		1.65	1 -1:C*C(R)*C*C*C*C*1 gem
		-0.32	1 -C-1:C*C*C*C*C*C*1 trans
H	6.39	5.25	1-ethylene
		0.09	1 -1:C*C(R)*C*C*C*C*1 trans
		1.05	1 -C-1:C*C*C*C*C*C*1 gem

Chapter 10: Pro Drawing Query Structures

What Are Query Structures?

Using a query structure to specify properties for atoms and bonds provides an efficient way to search chemical databases such as ChemFinder, DARC, RS^3, or ISIS/Base. You can use a query structure to narrow or broaden your search.

For example, creating a query structure indicating a bond as either double or single might broaden your search. Indicating atom properties where a particular atom must have a charge of +3 might narrow your search.

Because ChemDraw is not a chemical database application, the interpretation of query structures involves other programs. Not all databases support the same query properties. If you use a query structure containing properties not understood by a given database, one of the following may happen:

- An error message appears
- The unsupported properties are ignored

To use query structures for searching you may do either of the following:

- Paste the query structure into a database search window and initiate a search.
- Save the structure in an appropriate file format and open the file in the database application.

For more information on query properties see "Query Properties" on page 238, or consult the documentation for your chemical database.

NOTE: *ChemOffice 2005 does not prevent or warn you if you try to assign conflicting or nonsensical properties. For example, you can require that one of the atoms in benzene is not part of any ring, which is inherently impossible. The results of such a search depend on the query system used, but usually no matches are found.*

Atom Properties

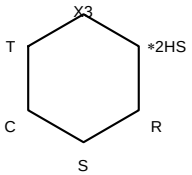
To assign properties to selected atoms in a structure:

1. Do one of the following:
   - Select a single atom by clicking it with a selection tool.
   - Select multiple atoms by Shift+clicking the atoms.
2. Then do one of the following:
   - Right-click, select the property you want, and then click the appropriate option.
   - From the **Structure** menu, choose **Atom Properties**. The Atom Properties dialog box appears.

- Press the Hotkey "*l*". The Atom Properties dialog box appears.

In the Atom Properties dialog box, select the properties to associate with the selected atom(s). Click **OK**.

Query indicators appear next to atoms that have associated atom properties.



The character that appears depends on which query properties have been assigned. If more than one property is assigned, more than one character appears adjacent to the atom. For more information, see "Query Indicators" on page 160.

The atom property indicators are shown in the following table.

Indicator	Query Property
*	Substituents: Free Sites (followed by the number of free sites)
U	Substituents: Up to (followed by the maximum number of substituents)
X	Substituents: Exactly (followed by the number of substituents)
H	Implicit Hydrogens
R	Ring Bond Count
S	Unsaturation
C	Reaction Change
T	Reaction Stereo
L	Translation
I	Isotopic Abundance
(none)	Abnormal Valence

Viewing Atom Property Values

Except for the three Substituents query properties, the characters indicate that a given property is applied, but not the value of that property.

To find the value of a query property setting:

1. Select the atom.
2. Do one of the following:
   - Right-click, point to an atom, and then point to the appropriate property.

- From the **Structure** menu, choose **Properties** and view the settings on the **Atom Properties** tab.

Removing Atom Properties

To remove all atom properties from an atom:

1. Select the atom.
2. From the **Structure menu**, choose **Properties**.
3. Click **Use Defaults**.

   The atom properties are removed and the characters no longer appear.

To remove specific atom properties:

1. Select the atom.
2. Do one of the following:
   - Right-click, point to an atom, point to the property you want, and then choose the appropriate option.
3. From the **Structure menu**, choose **Properties** and then click the atom property to remove.

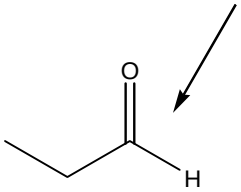
Atom Property Options

The following topics describe the atom properties you can associate with an atom.

Substituents

The three Substituents properties specify the number of substituents that may be bonded to the selected atoms. In ChemDraw, a substituent is defined as a non-hydrogen atom connected by a bond of any order.

For example, in the figure below, the carbonyl carbon, indicated by the arrow in propanal, has a substituent count of two: the alpha carbon and the aldehyde oxygen. The double bond to the aldehyde oxygen counts as only one substituent and hydrogen atoms never count as substituents.



The substituent count atom property allows you to specify the number of bonds to an atom in the target structure. This includes bonds already drawn in the query structure.

The substituent options are described in the following table.

Option	Search Result
Unspecified	*Default*. Search is determined by the target database. Some databases (including ISIS) find compounds with any substitution at this atom and some databases (including DARC) find only compounds with substitution exactly as drawn.

Option	Search Result
Free Sites	Finds compounds in which the selected atoms may contain a range of substituents up to the number specified plus the number of bonds as drawn. A value of zero finds a substituent count as drawn. You can also use the Free Sites symbol in the Chemical Symbols palette to apply free sites. For more information, see Chapter 6, "Drawing Orbitals, Symbols, Arrows, Arcs, and Other Shapes" on page 93.
Up to	Finds compounds in which the selected atoms may contain a range of substituents up to the number specified.
Exactly	Finds compounds in which the selected atoms contain the exact number of substituents as specified, up to 15 substituents.

Implicit Hydrogens

The Implicit Hydrogens property specifies whether additional, implicit hydrogen atoms may be attached to the selected atoms. If implicit hydrogen atoms are not allowed, all valences to that atom must be filled by bonds to non-hydrogen atoms. The implicit hydrogen options are described in the following table.

Option	Search Result
Allowed	*Default.* Finds compounds regardless of whether hydrogen atoms are attached to the selected atoms.
Not allowed	Finds compounds with no additional hydrogen atoms attached to the selected atoms.

Ring Bond Count

The Ring Bond Count specifies the number of bonds attached to an atom that are part of rings of any size. For simple cases, this also specifies the maximum number of rings in which an atom can reside. The ring bond count options are described in the following table.

Option	Search Result
Any	*Default.* Finds compounds in which the selected atoms can be a member of any type of ring, or a member of no ring at all.
No ring bonds	Finds compounds in which the selected atoms are acyclic.
As drawn	Finds compounds in which the selected atoms reside in the same type and number of rings as drawn.

Option	Search Result
Simple ring	Finds compounds in which the selected atoms is a member of only one ring (the atom has two ring bonds).
Fusion	Finds compounds in which the selected atoms lies at ring fusions (the atom has three ring bonds).
Spiro or higher	Finds compounds in which the selected atoms is a member of a spiro or higher linkage (the atom has four or more ring bonds).

Unsaturation

The Unsaturation property specifies whether a multiple bond is attached to the selected atoms. The unsaturation options are described in the following table.

Option	Search Result
Unspecified	*Default.* Finds compounds regardless of whether a multiple bond is attached to the selected atoms.
Must be absent	Finds compounds that do not have a multiple bond attached to the selected atoms.
Must be present	Finds compounds that have at least one multiple bond (double, triple or aromatic) attached to the selected atoms.

Reaction Change

The Reaction Change property specifies whether a change occurs at selected atoms after a reaction. This property is only meaningful when searching a database containing chemical reactions. The reaction change options are described in the following table.

Option	Search Result
May be anything	*Default.* Finds all reactions regardless of any change to selected atoms after a reaction.
Must be as specified	Finds all reactions that are changed at the selected atoms exactly as specified by the reaction center property in the Atom Properties dialog box.

Reaction Stereo

The Reaction Stereo property specifies that the selected atoms are stereocenters in a reaction. This property is only meaningful when searching a database containing chemical reactions.

The reaction stereo options are described in the following table.

Option	Search Result
Any	*Default.* Finds all compounds regardless of the stereochemistry at the selected atoms.
Inversion	Finds compounds in which the selected atoms have an inverted stereo configuration after a reaction.

Option	Search Result
Retention	Finds compounds whose selected atoms have an unchanged stereo configuration after a reaction.

Translation

The Translation property specifies what is required to match in the structure query and possible database hits in a Markush DARC query.

The translation options are described in the following table:

Option	Definition
Equal	*Default.* Matches specific to specific or generic to generic terms.
Broad	Translates specific query atoms to corresponding superatoms in the database.
Narrow	Translates query superatoms to corresponding specific atoms or groups in the database.
Any	Translates generic or specific terms to any term.

For more information, refer to the Markush DARC User Manual.

Isotopic Abundance

The Isotopic Abundance property gives you the ability to distinguish between different isotopic compounds—for example between mono- and hexa-deuterobenzene—by specifying a nuclide at any location.

The isotopic abundance options are described in the following table:

Option	Search results
Unspecified	*Default*
Any	For ChemFinder, the same as default. Included for compatibility with other systems where the default may be different.
Natural	Indicates an isotopically unmodified nuclide.
Enriched	Indicates a mixture of isotopically substituted and isotopically unmodified nuclides.
Deficient	Indicates a depleted label, that is, the nuclide is present in less than the natural ratio.
Nonnatural	Indicates an isotopically substituted nuclide, that is, essentially all the molecules of the compound have only the indicated nuclide.

Abnormal Valence

The Abnormal Valence property specifies whether selected atoms can have a valence other than normal. "Normal" valences for each element are defined in the Isotopes Table file in the ChemDraw Items folder.

NOTE: *The Abnormal Valence atom property does not provide a visual indicator.*

The Abnormal Valence options are described in the following table.

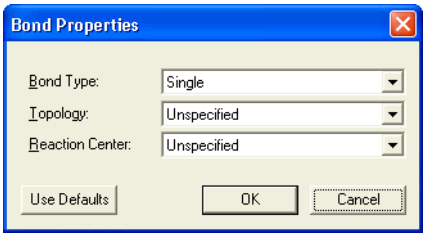
Option	Search Result
Not allowed	*Default.* Finds compounds where the selected atoms only have valences that are normal for that element. If necessary, hydrogen atoms are automatically added to or removed from the atom before transferring it to the chemical database. If the Check Structure When Copying to Clipboard or Exporting preference is turned on, an error message warns of abnormal valences.
Allowed	Finds compounds with the specific valence drawn.

NOTE: *If Abnormal Valence is Allowed, any Invalid Valence messages for those atoms are ignored automatically by the Check Structure command.*

Bond Properties

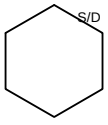
To define bond properties of selected bonds in a structure:

1. Do one of the following:
   - Select a bond using a selection tool.
   - Shift+click to select multiple bonds.
2. Then do one of the following:
   - Right-click, point to **Bond**, point to the property you want, and then choose the appropriate option.
   - From the **Structure** menu, choose **Properties**. On the **Bond Properties** tab, select the bond properties to associate with the selected bonds from the drop-down lists. Click **OK**.
   - Point to an bond and press the Hotkey "**/** ". The Bond Properties dialog box appears.

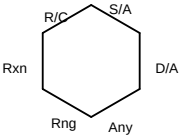


In the Bond Properties dialog box, select the properties to associate with the selected atoms. Click **OK**.

Query indicators appear next to bonds that have associated bond properties.



one bond



many bonds

The characters that appears depends on which query properties have been assigned. If more than one property is assigned, more than one descriptor appears adjacent to the atoms. For more information, see "Query Indicators" on page 160.

The indicators are described in the following table.

Indicator	Bond Query Property
Any	Bond Type: Any
S/D	Bond Type: Single/Double
D/A	Bond Type: Double/Aromatic
S/A	Bond Type: Single/Aromatic
Rng	Topology: Ring
Chn	Topology: Chain
R/C	Topology: Ring or Chain
Rxn	Reaction Center

Viewing Bond Property Values

The descriptor for the Reaction Center query property indicates that the property is applied, but not the value of the property.

To find the value of a query bond property setting:

1. Select the bond.
2. Do one of the following:
   - Right-click, point to the bond, and then point to the appropriate property.
   - From the **Structure menu**, choose **Bond Properties**, and view the settings of the drop-down list boxes.

Removing Bond Properties

To remove all bond properties from selected bonds:

1. Select the bonds.
2. From the **Structure menu**, choose **Properties**.
3. Click **Use Defaults**.

   The bond properties are removed and the indicators are no longer adjacent to the selected bonds.

To remove specific bond properties:

1. Select the bond.
2. Do one of the following:
   - Right-click, point to the appropriate property, and then click the property to remove.
   - From the **Structure** menu, choose **Properties**, and then click the bond property to remove.

Bond Property Options

The following are the atom properties that you can associate with an atom:

Bond Type

This property specifies the bond type of the selected bonds. The default bond type corresponds to the current type of the bond (single, double, etc.) as drawn.

The Bond Type options are described in the following table.

Option	Search Result
Single (all) and Dative	Finds compounds with the bond type you select for the selected bonds.
Double *or* Double Bold	Finds compounds whose selected bonds are double.
Double Either	Finds compounds whose selected bonds are double bonds and have either *cis/trans* stereochemical configuration.
Aromatic	Finds compounds whose selected bonds are aromatic.
Tautomeric	Finds compounds whose selected bonds are tautomeric.
Triple	Finds compounds whose selected bonds are triple.
Quadruple	Finds compounds whose selected bonds are quadruple.
Any	Finds compounds regardless of the bond type of the selected bonds.
S/D	Finds compounds whose selected bonds are single or double.
D/A	Finds compounds whose selected bonds are double or aromatic.
S/A	Finds compounds whose selected bonds are single or aromatic.

NOTE: *Not all bond types are supported in all file formats. When an unsupported bond type is saved to a given file format, it is converted to the closest equivalent that is supported.*

Topology

The Topology property specifies the ring environment of the selected bonds.

The Topology options are described in the following table.

Option	Search Result
Unspecified	*Default.* Finds compounds regardless of environment.
Ring	Finds compounds where the selected bonds are part of a ring.
Chain	Finds compounds where the selected bonds are part of a chain (and are specifically not part of a ring).

Option	Search Result
Ring or Chain	Finds compounds where the selected bonds are part of either a ring or a chain.

Reaction Center

The Reaction Center property specifies how the selected bonds are affected in a reaction. This property is only meaningful when searching a database containing chemical reactions.

The Reaction Center options are described in the following table

Option	Search Result
Unspecified	*Default.* Finds compounds regardless of whether the selected bonds are affected by the reaction.
Center	Finds compounds where the selected bonds are affected by a reaction, but the type of change is unspecified.
Make/Break	Finds compounds where the selected bonds are either broken or created in a reaction.
Change	Finds compounds where the bond order of the selected bonds changes in a reaction.
Make& Change	Finds compounds where the selected bonds are formed, broken, or undergo a change in bond order.
Not Center	Finds compounds where the selected bonds are not part of the reaction center.
Not Modified	Finds compounds where the selected bond's orders do not change, but which may or may not be part of the reaction center.
Unmapped	Finds all compounds.

3D Properties

3D queries are particularly useful in pharmacophore searching where the user is looking for a particular 3D relationship among atoms and bonds, for example in a series of potential receptor ligands. To create a 3D query, you add geometries (lines, planes, etc.) and constraints (specified as ranges) to a query structure. For example, you might specify that two atoms must be between 4 and 5 Å apart, or that two planes must be separated by 80-100 degrees.

To assign 3D properties to a structure, select the structure or sub-structure and then select one of the following options from the **Add 3D Property** entry on the Structure menu.

NOTE: *Because some 3D properties specify an order, you should use Shift+Click to select them in the proper order rather than using the Marquee or Lasso tool to select them all at once.*

In the table below, *points* are may be atoms, centroids or points. *Lines* may be lines or Normals.

Option	Search Result
Angle	Defines an angle constraint between three points (in order). Indicated as a range.
Dihedral	Defines a dihedral (torsional) angle constraint among four points (in order), between two lines, or two planes. Indicated as a range.
Distance	Defines a distance constraint between two points, a point and a line, or a point and a plane. Indicated as a range, in Angstroms.
Line	Defines the best-fit line for the selected points.
Plane	Defines the best-fit plane for the selected points, or for a point and a line.
Exclusion Sphere	Defines an exclusion sphere around a point. If more than one point is selected, the exclusion sphere is around the first selected point, and the subsequent points are allowed within the exclusion sphere when the query is evaluated. Indicated as a range, in Å, beginning at 0.
Normal	Defines the normal from a defined plane in the direction of a point.
Point	Defines a point positioned at a specified distance from a first point in the direction of a second point (in order), or in the direction of the normal.
Centroid	Defines a point positioned at the average position of all other points selected.

All constraint values can be edited with the text tool. Only exclusion spheres show the change visually.

When you create a point, a dialog box is displayed. Specify the distance from the first selected point to the calculated point. The distance may be specified as an absolute value in Å or as a percentage of the distance between the selected points. Negative values indicate that the calculated point is further from the second point than the first point is, rather than being between them.

Geometry and constraint objects update dynamically when you change the structure; they cannot be moved independently. They may be used with .cdx, .mol, .skc, and .tgf files (full read-write compatibility); they are not compatible with other formats. They can, however, be saved in print-only formats such as TIFF.

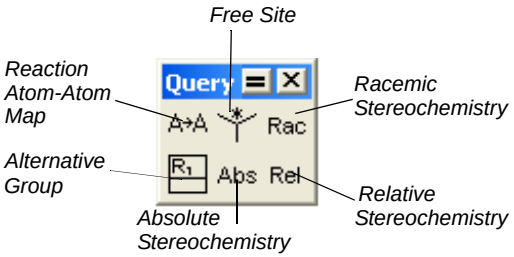
Query Tools Palette

ChemDraw provides Query tools to enable you to draw query structures.

To display the Query tools, select **Show Query Tools** from the **Other Tools** entry on the View menu, or click the Query Tools icon on the Main Tool Palette:

- Click .

  The Query tools palette appears.



Query Indicators

You can display small characters to indicate query properties you assign to atoms and bonds.

Viewing Query Indicators

To display query indicators for a structure:

- Select a structure to which query indicators are assigned, right-click, point to **Atom** or **Bond**, and then click **Show Query Indicator**.

To display query indicators for individual atoms or bonds:

- Select the atom or bond, right-click, and choose **Show Query Indicator**.

Hiding Query Indicators

To hide an individual indicator:

1. Select the indicator to hide.
2. Right-click and select **Hide Indicator**.

Removing Query Indicators

To delete a query indicator:

1. Click the indictor.
2. Click the eraser tool and then click the indicator.

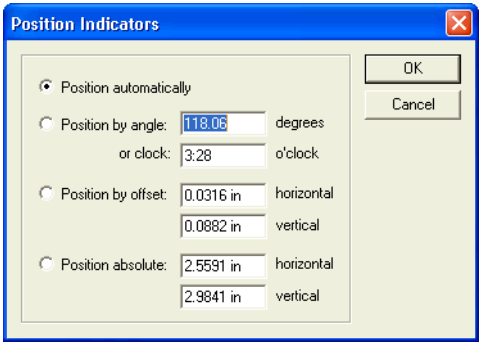
Positioning Query Indicators

Query indicators are positioned automatically and move appropriately if a structure is modified. You can reposition them by dragging them to the desired position or with the Indicator Position dialog box.

To reposition an indicator numerically:

1. With a selection tool, click the indicator to move.
2. Right-click and choose **Position**.

   The Position Indicator dialog box appears.



3. Click the appropriate Position option, and type a value:

To Position ...	Type a value for...
from the atom or bond center to indicator center	angle, degrees or clock, o'clock

To Position ...	Type a value for...
from the atom or bond center to bottom left of indicator baseline	offset, horizontal and vertical
at specified coordinates	absolute, horizontal and vertical

Drawing Stereochemical Symbols

ChemDraw provides three types of stereochemical flags that indicate that the molecule with which they are associated represents one of the following:

- **Racemic**—A racemic mixture.
- **Absolute**—A pure enantiomer of known configuration.
- **Relative**—A pure enantiomer of unknown configuration.

The font and size for stereochemical flags is determined by the default Atom Label size for the document.

To draw a stereochemical flag:

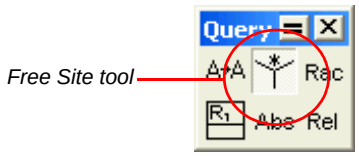
1. On the Query tools palette, click the tool for the flag you want to use.
2. Position the pointer next to the structure to which you want to assign the flag.
3. Click to deposit the symbol.

Drawing Free Sites

Use the Free Sites tool to increment or decrement the number of free sites in a query structure.

To increment the number of Free Sites:

1. On the Query tools palette, click the **Free Site** tool.



2. Position the pointer over the atom to which you want to apply free sites.
3. Click to add the symbol.
4. Continue to click the atom to increment the free site number.

To decrement the number of free sites:

- Hold the **Alt** or **Option** key while clicking the atom.

You can also change the free sites by using the Atom Properties dialog box or the shortcut menu. For more information see “Atom Properties” on page 149.

Generic Nicknames

Generic nicknames represent a class of elements or structural moieties. For example:

- “M” can be a generic nickname for all metals
- “X” can represent halides
- “Ary” can represent an aromatic substructure

If you are using a query system that recognizes generic nicknames, you can use these nicknames in your ChemDraw query structure.

You can assign Generic nicknames, like other nicknames, to HotKeys. For information on assigning a Hotkey to a nickname, see Chapter 9: “Working With Structures”.

You cannot define the *meaning* of a generic nickname in ChemDraw because generic nicknames represent multiple (and perhaps an

infinite number of) substituents. Generic nicknames have meaning only in the context of the search system you are using.

The generic nicknames recognized as chemically meaningful to ChemDraw are listed in Generic Nicknames file in the ChemDraw Items folder. For definitions of the nicknames, see "Nickname Definitions" in the Help file.

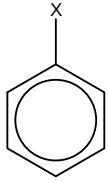
To edit the generic nickname files:

Open the Generic Nicknames file in a text editor and make your changes.

See the provided Generic Nicknames file for examples of the correct format.

To label an atomic position with a generic nickname, use the same procedures as labeling an atom:

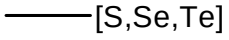
1. Do one of the following:
   - Open a text box on an atom position by clicking with the **Text** tool.
   - Double-click on an atom position with a Bond tool.
2. Type the generic nickname.
3. Press **Return** or click outside the text box.



NOTE: *If you perform Check Structure on a structure with a generic nickname, a message is displayed because the structure contains variable substituents. If you ignore this message, the generic nicknames are ignored and ChemDraw reports the chemical formula, mass, and so on as if the atom label containing the generic nickname were not selected.*

Element Lists

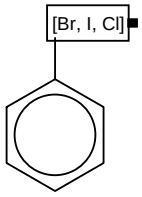
You can define your search query more concisely with the element list. By labeling an atom position as a list of elements you specify that one of these elements must match in the structure for which you are searching. The elements in the element list must be separated by commas. A space after each comma and brackets are optional. An example of an element list is shown below.



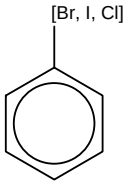
NOTE: *An element list may contain only atomic symbols, plus D (deuterium) and T (tritium).*

To create an element list:

1. Open an atom label text box.
2. Type an open bracket ("**[**") followed by a list of elements separated by commas ("Cl, Br, I"), followed by a close bracket ("**]**").



3. Close the text box.

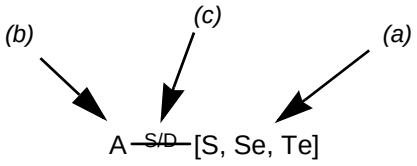


The following example shows a query structure created to find compounds matching the following criteria:

a. Non-oxygen chalcogenide bonded to another atom.

b. Not necessarily carbon (a generic nickname).

c. The bond type between the chalcogenide and the other atom to be a single or double bond.



The "A" label indicates that the atom may match any atom except hydrogen. The mark near the bond indicates that the bond has special properties. The bond type specified in the Bond Properties dialog box must be single or double, S/D. The "[S,Se,Te]" specifies that one of these elements must match in the target structures.

Element Not-Lists

The element not-list specifies that the elements in the list match must not match in the structure for which you are searching. Commas must separate the elements in the element not-list. A space after each comma and brackets are optional.

The word NOT must be in all-caps and must be followed by a space. Alternatively, the word NOT may be replaced with a minus sign.

For example:

NOT[F,Cl,Br]	[NOT C,O,N]
NOT[F,Cl,Br,I]	*[NOT C,O,N]*

NOTE: *An element not-list may contain only atomic elements, plus D (deuterium) and T (tritium).*

To create an element not-list:

1. Open an atom label text box.
2. Type an open bracket, the word NOT, and a space ("[NOT") followed by a list of elements separated by commas ("Cl, Br, I"), followed by a close bracket ("]").

Link Nodes

You can specify a variable-length chain or ring by indicating that one of the atoms can be repeated some number of times using link nodes.

Link nodes must have exactly two connecting bonds. The atom label must conform to the following conditions:

- No more than a single element symbol or a generic nickname
- The last part of the label in the form: *number hyphen number,* with the number and hyphen subscripted
- Parentheses or braces may be used instead of brackets
- Brackets can be omitted if not needed for clarity, for example with $O_{1\text{-}3}$

To create a link node:

1. Open an atom label text box.
2. Type in the following format:

$[CH_2]_{3\text{-}7}$

Representing Polymers and Other Repeating Units

Brackets, parentheses, and braces enclose structures or structural fragments that are to be repeated a number of times. The bracket properties in ChemDraw allow you to specify the context and orientation of the repeating units.

To enclose structures with brackets:

1. Click the **Bracket** tool and select one of the double bracket tools.
2. **Click+drag** across the structure to draw the brackets.
3. **Right-click** or **Control-click** and select the appropriate bracket properties from the menu that appears.

The bracket properties are described in the following sections.

NOTE: *This method will give a default value for component order, multiple group repeat count, or SRU label. To change a default value, use the Bracket Properties dialog box.*

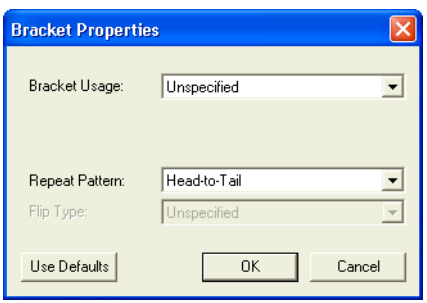
Setting Bracket Properties

You can change the properties of brackets by the context menus or Bracket Properties dialog box.

To use the Bracket Properties dialog box:

1. Select the right bracket with a selection tool.
2. From the Structure menu, choose Bracket Properties.

   The Bracket Properties dialog box appears.



The Flip Type option appears only for brackets with exactly two crossing bonds, and is disabled in other cases.

You can customize the text that appears to the bottom right of the bracket for the following bracket types.

- Component (c#)—the Component Order must be a non-negative integer, and is displayed as the letter "c" followed by that integer (or "c" alone if an order of zero is specified).
- Multiple Group (#)—the Repeat Count must be a positive integer.
- SRU (n)—the SRU label can be any text.

You can also edit the text for these Bracket Usage types directly in the document using the Text tool. You cannot edit the text displayed for the other Bracket Usage types.

Bracket Usage

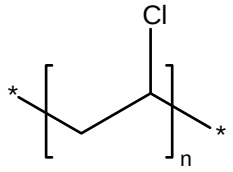
Representations of polymers are either structure-based or source-based. The type of bracket you use depends on which type of representation you need. For references, see "Polymer Representations" on page 238.

Structure-based Polymer Representations

Structure-based polymer representations enclose only a portion or a structure within brackets. One or more bonds cross each of the enclosing brackets. The crossing bonds "match up", making the polymer structure more explicit.

You create a structure-based polymer representation by enclosing a portion of a structure in brackets with a bracket type of SRU (n). The subscript "n" is recommended by IUPAC to notate structure-based representations of unknown size, but you can edit the text using the text tool.

A structure-based representation of poly(vinyl chloride) is shown below.



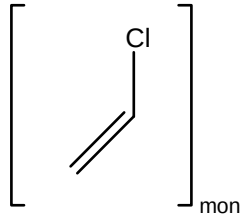
You can also use the Bracket Usage types "Crosslink (xl)", "Graft (grf)", and "Modification (mod)" to represent specific types of repeating units in a structure-based representation, but they are rarely encountered and using them is discouraged.

Source-based Polymer Representations

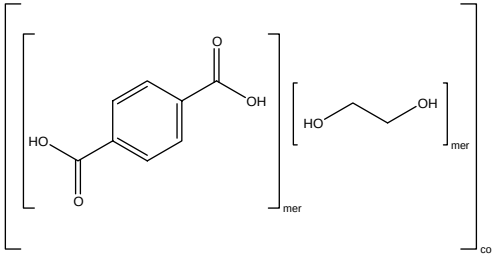
Source-based polymer representations enclose an entire discrete chemical substance in brackets. The mode of polymerization may be obvious from context, or it might be unknown. Source-based representations are useful when describing processes where the starting materials are known, but the exact structure of the reaction product is not.

You can create a source-based representation by enclosing a structure in "Monomer (mon)" brackets.

A source-based representation of poly(vinyl chloride) is shown below.



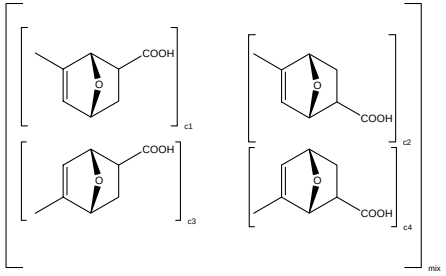
You can use "Mer (mer)" brackets for components of a copolymer where those individual components are known not to repeat themselves or alternate with the other components. An example is shown below.



Copolymers represent substances with more than one repeating unit. In general, you can use bracket type "Component (co)". You can also use "Copolymer, alternating (alt)", "Copolymer, random (ran)", and "Copolymer, block (blk)" to represent different specific types of copolymers in a source-based representation, but they are rarely used and their use is discouraged.

The bracket type, "Mixture, unordered (mix)" is not for polymers, but to represent a collection of substances that may all be present, but not necessarily in known amounts. Bracket type "Component (c)" indicates individual mixture elements.

An example is shown below.

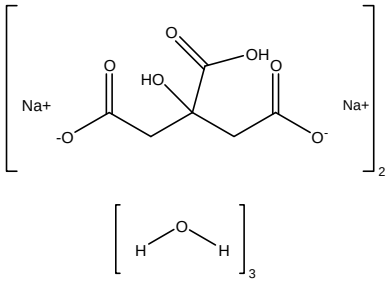


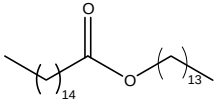
Bracket type "Mixture, ordered (f)" is primarily used to describe manufacturing processes, where the ordering of components is a critical part of the

process (and where a different ordering might produce a different final product. As with Unordered Mixtures, individual elements of an ordered mixture should be surrounded by brackets with a bracket usage of "Component (c)". Unlike with Unordered Mixtures, however, components of Ordered Mixtures must represent their ordering. You can do this by editing the "c" label with the text tool to include a number ("c1", "c2", and so on.)

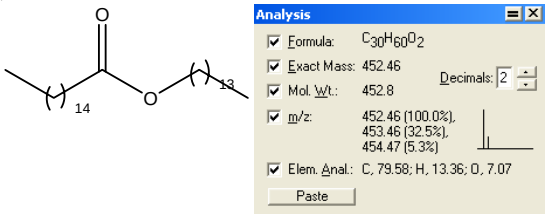
You use the bracket type, "Multiple Group (#)" to indicate that the enclosed items are repeated a specific known number of times. Multiple Group brackets may enclose entire structures, or may enclose a portion of the structures only. You can edit the numeric repeat count with the text tool.

Examples follow.





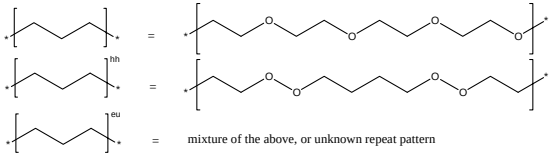
Because Multiple Group brackets represent a specific repeat count (unlike the unknown repeat count of the other bracket types), it is possible to calculate accurate molecular weights (and related data) for such structures. That data is displayed in the Analysis window as with any other structure.



Repeat Pattern

For simple linear polymers, the repeating units may connect head-to-tail or head-to-head (or their repeat pattern might be a mixture or unknown). You can also assign this property to brackets.

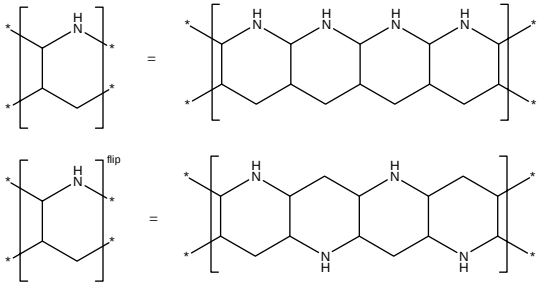
Because of its prevalence, the Head-to-Tail type is assumed to be the default Repeat Pattern, and does not receive any special annotation on the brackets, as shown below.



Flip Type

For ladder-type polymers (those polymers with two connecting bonds on each side), there is a potential ambiguity in the order of the connections. You can assign the Flip Type property to resolve that ambiguity. This property is appropriate only for brackets with exactly two crossing bonds, and is disabled in other cases.

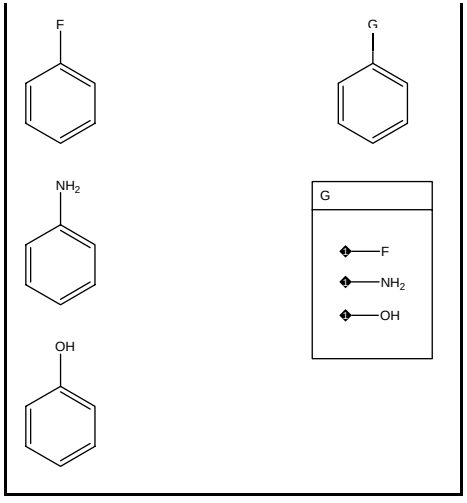
Because of its prevalence the No Flip type does not receive any special annotation.



Alternative Groups

You can create a search query that contains variable functional groups or substructures. Instead of submitting multiple queries on structures that share a common substructure, you can submit a single query with the parent structure. The parent structure can have attachment points to a list of alternative groups that you can define.

Alternative groups, sometimes called R-Groups or G-Groups (Generic Groups), are shown below.



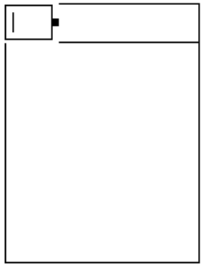
Defining an Alternative Group

In ChemDraw Pro, you can create alternative group definitions (R, G, etc.) that represent a set of substituents, any one of which will match the query.

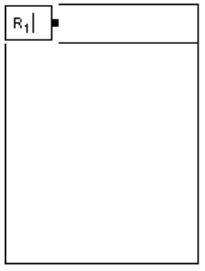
To define an alternative group:

1. Click the **Alternative Group** query tool R_1.
2. Click and drag to create an area large enough to draw the alternative groups.

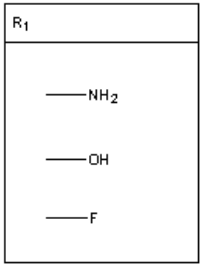
   The Alternative Group Title box appears.



3. Type a title, such as R_1, in the Alternative Group Title box.



4. Draw the substructure fragments in the Alternative Group box.

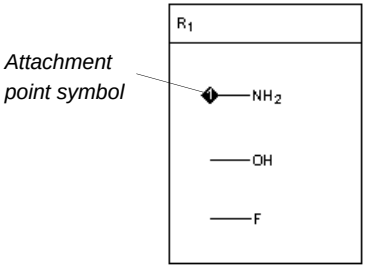


Defining Attachment Points

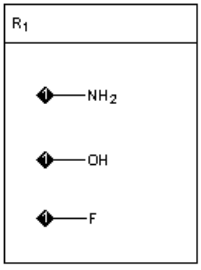
Specify where the fragments should bond to the parent structure at the alternative group label:

1. Click the diamond shaped **Attachment Point** tool on the Chemical Symbols palette.
2. Do one of the following:
   - Click a substructure fragment where you want to place the attachment point.
   - Point to a substructure fragment where you want to place the attachment point and press the Hotkey "**.**".

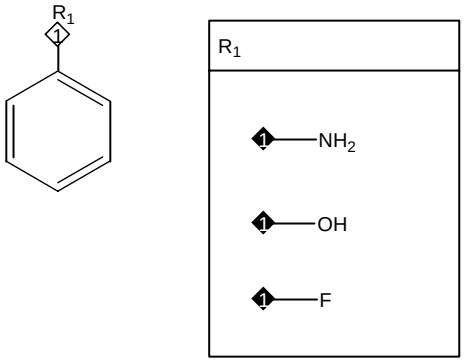
   An attachment point symbol appears.



3. Repeat step 2 for all fragments.



When you create a parent compound that contains an alternative group you defined, an attachment point symbol appears next to the label. The attachment point number matches that found in the definition.

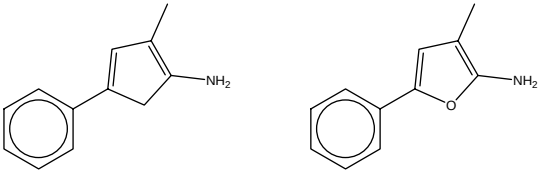


The number displayed in the attachment point symbol is the attachment rank order. See the example in "Multiple Attachment Points" on page 168.

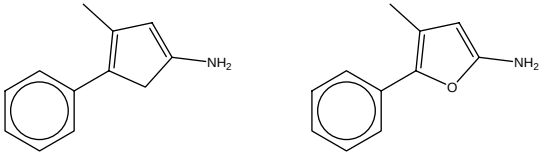
Multiple Attachment Points

If you have well-defined multiple attachment points on your structure fragments, you can perform searches for specific materials. This type of search is especially useful for searching for conformationally similar structures.

For example, you want to find the two compounds below:



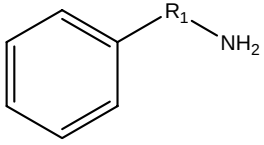
However, you are not interested in the two compounds below:



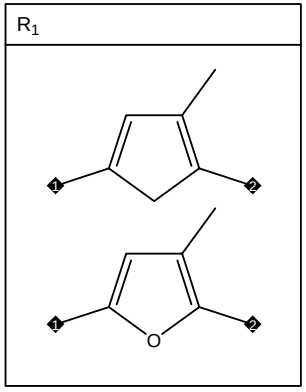
By specifying the attachment points order, you can exclude the unwanted compounds. The parent structure below satisfies the necessary requirements.

To specify the attachment points order:

1. Draw the parent structure shown below.



2. Create an Alternative Group Box labeled "R1".



3. Draw the structure fragments and label them with attachment points.

   When the alternative group definition is complete, the attachment point symbols appear in the parent compound.

By numbering your attachment points, you have unambiguously specified that the methyl group must be adjacent to the amine group. The conformations that are not of interest are excluded.

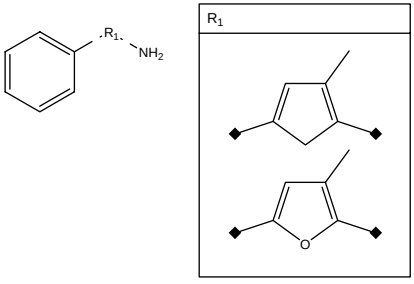
Showing Attachment Rank Indicators

You can hide the attachment rank indicators if required. For example, sometimes—particularly in publication-quality drawings—the numbering of attachment points is implicit and the numbered attachment rank indicators are superfluous.

To hide the attachment rank indicators and remove the numbers from the attachment points:

1. From the **File** menu, choose **Preferences**.
2. In the **Preferences** dialog box, click **Display**.
3. Deselect **Show Attachment Rank Indicators**.

The following illustration shows an alternative group definition and a parent structure with the attachment rank indicators hidden.



This change affects all documents.

Attachment Point Numbering

Numbered attachment points allow you to specify precisely how the structure fragments are connected to your parent structure.

The numbering of the attachment points is related to the front to back order of the attachment points.

To set the order of the attachment points:

- Click the ends of the bonds in order.

  The last point clicked has the highest number.

To change the ordering of the attachment points do one of the following:

- Click the attachment points with the **Attachment Point** tool.
- Select an attachment point with a selection tool, and from the **Object** menu, choose **Bring to Front** or **Send To Back**.

  The attachment point numbers are highest in the front.

Lists

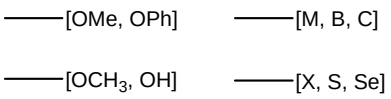
You can use an R-Group table to construct a list of molecules.

Anonymous Alternative Groups

An anonymous alternative group is a cross between an element list and an alternative group. Element lists are restricted to single elements, but anonymous alternative groups can contain any structure that can be represented by text. Nicknames and generic nicknames are allowed in anonymous alternative groups. Anonymous alternative groups are shortcut notation for regular alternative groups, eliminating the need to specify a name such as "R1".

You can define your search query more concisely with the anonymous alternative group. By labeling an atom position as a list of substructures you specify that one of these substructures must match in the structure for which you are searching. Commas must separate the items in the anonymous alternative group. A space after each comma and the brackets are optional.

Examples of anonymous alternative groups follow:



To create anonymous alternative groups:

1. Open an atom label text box.
2. Type an open bracket "**[**"followed by a list of elements, fragments, nicknames, or generic nicknames separated by commas, followed by a close bracket "**]**".

Atom-to-Atom Mapping

You can create correspondences between atoms in different structures for use in creating queries for searching a reaction database. The reactions mapped can be single or multi-step. You can assign atom-to-atom mapping for creating records for a reaction database and for creating queries for searching a reaction database. You can assign atom mapping in two ways:

- Automatic mapping, using the **Map Reaction Atoms** command from the **Structure** menu.
- Manual mapping, using the Reaction Atom-Atom Map tool on the main tools palette.

During either type of mapping process, the mapping algorithm perceives and assigns a reaction center for the reactants and products.

When a reaction map is established, you can point to an atom in one structure with the Reaction Atom-Atom Map tool selected to highlight the mapped atom in the other structure.

Always Display and Print Atom Mapping

To make the symbols always appear and print on the atoms when reaction mapping has been performed:

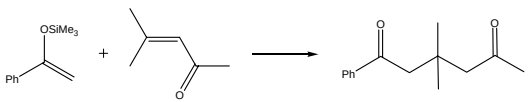
1. From the **File** menu, choose **Preferences**.
2. In the Preferences dialog box, click **Display**.
3. Select **Always Display and Print Reaction Mapping**.
4. Click **OK**.

Deselect Always Display and Print Atom Mapping to show the symbols only when you select the Reaction Atom-Atom Map tool. When this option is deselected, atom mapping symbols do not print, even though a reaction map has been created.

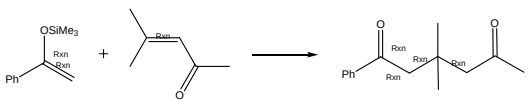
Automatic Mapping

To automatically create a reaction map:

1. Draw the reaction you want to map. For example:



2. Select the reactants and products in the reaction.
3. From the **Structure** menu, choose **Map Reaction Atoms**.

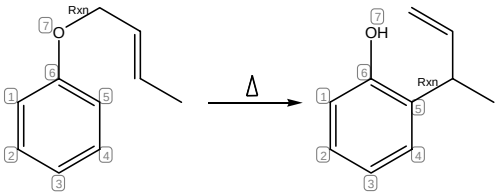


The symbol "Rxn" appears next to the bonds in the reactant and product that are perceived by the algorithm as being modified by the reaction. These symbols are bond properties that are automatically applied. For more information about the Reaction Center bond property, see "Bond Properties" on page 155.

Manual Mapping

In situations that require manual mapping of atoms, you can use the Reaction Atom-Atom Map tool. This might be necessary when the automatic mapping is applied to complicated reactions. In these cases you can manually readjust the reaction mapping.

The following figure shows how to amend the initial mapping by using the Reaction Atom-Atom Map tool.



When you perform manual mapping with the Reaction Atom-Atom Map tool, you can suppress automatic re-mapping of atoms other than your target atom.

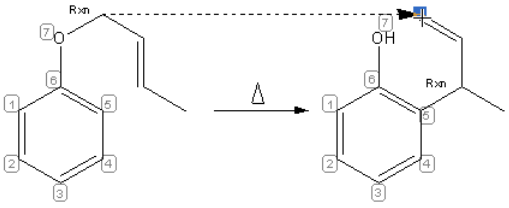
To suppress automatic re-mapping:

1. From the **File** menu, choose **Preferences.**
2. On the General tab, select **Automatic Reaction Mapping**.
3. Click **OK**.

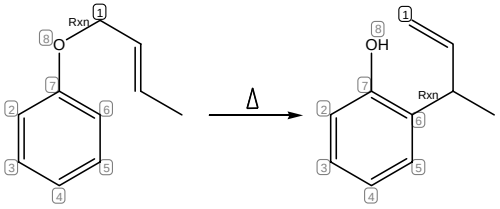
To use the Reaction Atom-Atom Map tool to supplement the automatic mapping:

1. Click the **Reaction Atom-Atom Map** tool A→A .
2. Point to the atom in the reactant whose mapping you want to establish. For example, in the following drawing you would point to the acyclic carbon adjacent to the ether oxygen.

3. Drag from the reactant atom to the corresponding product atom.



The remaining atoms are automatically mapped based on the manual mapping you performed.



You can continue to set or change the mapping for other atoms in the reaction if necessary until you get exactly the mapping you want. For this example additional manual mapping is not necessary.

Clearing Reaction Mapping

To clear all reaction mapping:

1. Select the structures whose mapping you want to remove.
2. From the **Structure** menu, choose **Clear Reaction Map**.

Exporting Reaction Mapping

Reaction mapping and reaction center perception information are stored in the native ChemDraw file format (*.cdx) for reopening in ChemDraw and the ISIS Reaction file format for transfer to other applications that read atom mapping, such as ChemFinder and ISIS/Base. You can also copy mapped reactions to these same applications using the Clipboard.

Export Compatibility

Because query properties are only useful in a chemical database, you must transfer your structures from ChemDraw into your search system. Not all file formats support the same query properties and not all chemical databases support the same file formats. Consult the documentation for your database to see which file formats are supported.

The following table lists the query properties that ChemDraw writes to ISIS (SKC, TGF, and Clipboard) file formats. All query properties are written to the ChemDraw (CDX) file format. CDX is the preferred format to use to retain all query properties in a drawing.

Exported Query Properties	**ISIS**	**Mol**	**Rxn**
Atom Properties			
Substituents			
Unspecified	**X**	**X**	**X**
Free Sites	b	b	b
Up to	a	a	a
Exactly	**X**[c]	**X**[c]	**X**[c]
Implicit Hydrogens			
Not allowed	**X**	**X**	**X**

Exported Query Properties	ISIS	Mol	Rxn
Allowed	X	X	X
Ring Bond Count			
Any	X	X	X
No ring bonds	X	X	X
As drawn	X	X	X
Simple ring	X	X	X
Fusion	X	X	X
Spiro or higher	X	X	X
Unsaturation			
Unspecified	X	X	X
Must be absent			
Must be present	X	X	X
Reaction Change			
May be anything	X		X
Must be as specified	X		X

Exported Query Properties	ISIS	Mol	Rxn
Reaction Stereo			
Any	X		X
Inversion	X		X
Retention	X		X
Translation			
Equal			
Broad			
Any			
Narrow			
Abnormal Valence			
Not Allowed	X	X	X
Allowed	X	X	X
Bond Properties			
Bond Type			
Single	X	X	X
Dashed	X	X	X
Hashed	d	d	d

Exported Query Properties	ISIS	Mol	Rxn
Wedged Hashed	X	X	X
Bold	X	e	e
Wedged	X	X	X
Wavy	X	X	X
Hollow Wedged	e	e	e
Dative	f	f	f
Double	X[g]	X[g]	X[g]
Double Either	X	X	X
Double Bold	h	h	h
Aromatic	X	X	X
Tautomeric	i	i	i
Triple	X	X	X
Quadruple	l	l	l
Any	X	X	X
S/D	X	X	X
D/A	X	X	X
S/A	X	X	X
Topology			
Unspecified	X	X	X
Ring	X	X	X
Chain	X	X	X
Reaction Center			
Unspecified	X		X
Center	X		X
Make/Break	X		X
Change	X		X
Make&Change	X		X
Not Center	X		X
Other Query Attributes			
Generic Nicknames	X[j]	X[j]	X[j]
Element Lists	X[ko]	X[ko]	X[ko]
Element Not-Lists	X[k]	X[k]	X[k]

Exported Query Properties	ISIS	Mol	Rxn
Alternative Groups	**X**	**X**[m]	
Anonymous Alternative Groups	n	n	
Link Nodes	p	p	p
Bracket properties	**X**	**X**	**X**
Atom-Atom mapping	**X**		**X**
Variable Attachment Positions			
3D query properties			

[a] Converted to the appropriate number of exact substituents

[b] Free Sites counts of zero translated to "Substitution as drawn"; all other Free Sites values written as substitution counts equal to the total current valence plus the free sites value.

[c] Substituent counts of greater than 5 are translated to "6 or more"

[d] Converted to Wedged Hashed

[e] Converted to Wedged

[f] Converted to a Single, with a positive charge applied to that atom at the base of the dative bond and a negative charge applied to the atom at the point of the dative bond

[g] Interpreted by ISIS as unspecified *cis/trans* stereochemistry

[h] Converted to Double

[i] Converted to S/D

[j] Only M, X, Q, A; others written as aliases

[k] Truncated to the first 5 elements

[l] Converted to single.

[m] An RGFile will be created automatically.

[n] Converted to non-anonymous alternative groups.

[o] Lists of greater than 5 elements converted to alternative groups.

[p] The low end of the repeat range is always treated as 1.

Chapter 11: Working With Page Layout

Overview

The presentation quality of your ChemDraw document is determined by how well the chemical structures and other objects are placed on the page (layout). Effective layout of a drawing includes proper alignment of chemical structures and other objects, appropriate page size, and page orientation. The page layout tools include: setup of the page and the use of the ruler, and the grouping, layering, aligning, and distributing commands. You can also organize information on the page using tables.

Controlling the Drawing Area

The size of a document window is not necessarily the same as the size of the drawing area of the page. A document window, in most cases, actually covers only a portion of the drawing area.

The following options allow you to set the drawing area displayed on your screen.

- Document Settings and Page Setup from the File menu allow you to set the size and orientation of the page, margins, headers, footers, and the document type and size.
- View menu options: Actual Size, Fit to Window, Magnify, and Reduce.
- Magnification Controls: enlarge and reduce
- Dragging to enlarge the drawing area.
  - **Windows:** Point to a border or corner of a document window and drag to resize.
  - **Macintosh**: Drag the Size box in the lower right corner of the document window.

The size of drawing area displayed depends on the size and resolution of your monitor. In some cases you can see the entire document.

If you magnify a document, the drawing area size and drawing objects become bigger. If you increase the magnification so that the page size becomes bigger than the screen, scroll bars become available.

Setting up Pages

You can create two types of documents:

Pages—A single document containing one or more sheets, each of which is printed on a single piece of paper.

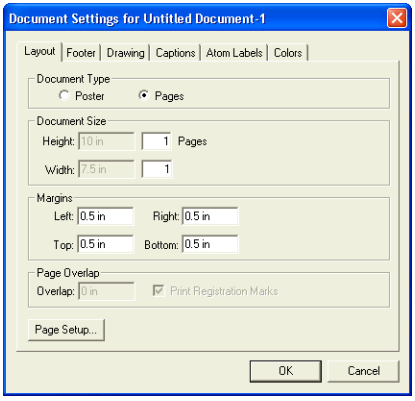
Posters—A single large document, composed of as many pieces of paper as necessary.

Paged Document Setup

To create a document with one or more page:

1. From the **File** menu, choose **Document Settings**.

   The Document Settings dialog box appears.



2. On the **Layout** tab, ensure **Pages** is selected.
3. Specify the number of pages in the Document Size section.

   The size of the pages is determined by the Page Setup settings. For more information, see "Page Setup" on page 179.
4. Type the **Margin** settings.

   The units of the margins are set in the Preferences dialog box. The paper size minus the margins determines the drawing area.
5. Create Headers and Footers as described in "Creating Headers and Footers" on page 178.
6. Click **OK**.

   A document is created using your settings.

Poster Documents Setup

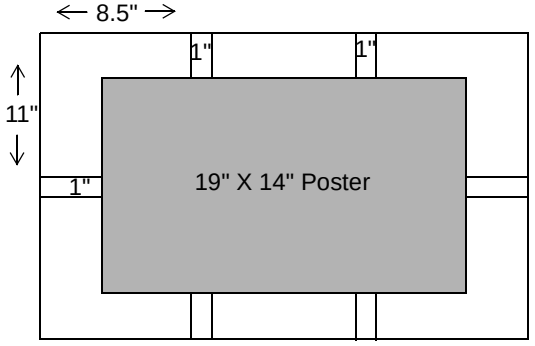
You can create a poster by creating a single large drawing area, which will be printed on as many separate pages as necessary. When you set the document size and how much each page overlaps, ChemDraw calculates the number of pages needed and the margin sizes. You can set registration marks, which mark the overlap setting on each page, to use as a guide when assembling the poster from the separate pages.

To create a poster document:

1. From the **File** menu, choose **Document Settings**.
2. On the Layout tab, click **Poster**.
3. Type the **Height**, **Width**, and **Page Overlap**.

   The number of pages and the margin dimensions are calculated.
4. Select whether to **Print Registration Marks**.
5. Create Headers and Footers as described in "Creating Headers and Footers" on page 178.
6. Click **OK**.

An example of a 19-inch by 14-inch poster, consisting of six 8.5-inch by 11-inch pieces of paper with a 1-inch overlap is shown below.

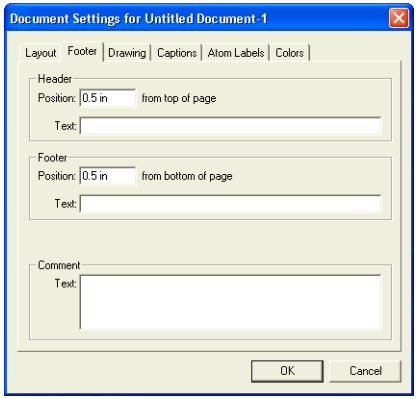


Creating Headers and Footers

You create headers and footers in the Document Settings dialog box. In poster documents, only one header and footer appear for the entire document.

To create headers and footers:

1. From the **File** menu, choose **Document Settings**.
2. Click the **Footer** tab.



3. Type the value of the position from the edge of the page that you want the header or footer to appear.
4. Type the text to appear in the header or footer.
5. Type additional information in the **Text** box from the following table:

To include the...	Type ...
file name	&f
page number	&p
date printed	&d
time printed	&t

6. Position the text horizontally by typing the characters in the table below. Any text following these characters is appropriately aligned.

To align the text ...	Type ...
centered	&c
right	&r
left (default)	&l

Page Setup

The Page Setup parameters that affect the size of the drawing area are:

- Page size
- Orientation

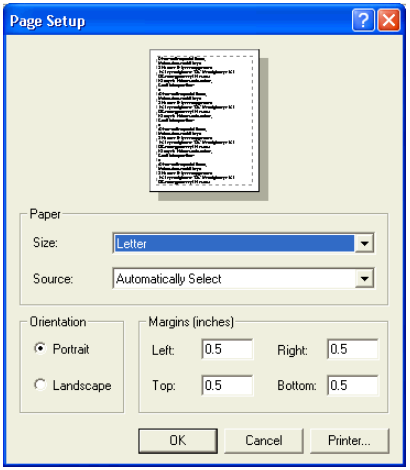
These parameters are specified in the Page Setup dialog box. The Page Setup dialog box and the options available vary depending on the printer you have chosen. For the Macintosh, the version of the printer driver for that printer is installed in your System Folder.

To set the paper size, orientation, and margins:

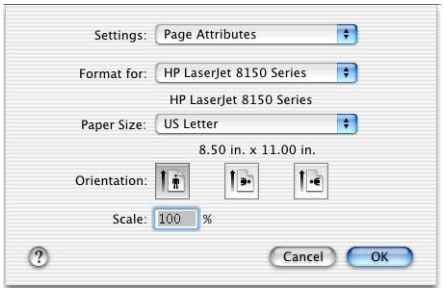
1. From the **File** menu, choose **Page Setup**.

   The Page Setup dialog box appears. The dialog box appears slightly different depending on the printer and platform you have.

A Windows dialog box for a typical postscript printer is shown below.



The Macintosh Page Setup dialog box with common settings for a LaserWriter is shown below.



2. Select a paper size from the drop-down list.

   The available page sizes vary depending on the type of printer. Listed below are common sizes available. The page orientation you choose determines which of the measurements is height and which is width:

Paper Type	Dimensions
US Letter	8.5 x 11 inches
US Legal	8.5 x 14 inches
A4 Letter	21 x 29.7 cm
B5 Letter	17.6 x 25 cm
Tabloid	11 x 17 inches
International	8.5 x 12 inches
Computer	14 x 11 inches

Page Orientation

To choose the orientation of the page:

- Click the vertical (portrait) or horizontal (landscape) orientation button.

  The orientation of a document window changes to the orientation you have chosen. This is evident when the rulers are visible.

Reduce or Enlarge

Some printers include an option to reduce or enlarge your drawings by a variable percentage (25-400%). This option scales all objects and text in the document window by the percentage specified. This is not a change in magnification. The size of objects is changed relative to the paper size, margins, and orientation you have specified.

The enlarge or reduce option is useful for changing the size of the available drawing area, while keeping the images on the screen at the normal size when you are drawing. If your document is set so that the drawing fills the page on one printer and you use another printer that requires larger margins, the drawing my disappear off the edge of the document window. You can reduce the size of the drawing with the reduce option so that it fits in the document window.

Saving Page Setup Settings

You can save Page Setup settings in a Style Sheet or Stationery Pad. Whenever you open a Style Sheet or Stationery Pad, these settings are automatically used. The Page Setup settings are saved in addition to the Text settings, Drawing Settings, and the Color Palette.

35mm Slide Boundary Guides

If you make 35mm slides from a hard copy of a ChemDraw document or from a screen shot, you can display boundary lines that appear on your screen positioned at 7 inches and 10.5 inches to match the 2:3 ratio for the 35 mm slide format. These guides help you keep your drawing within this region to maintain the proper ratio, but are not printed. The drawing area of the page must be at least 7 x 10.5 inches for these boundary lines to be visible.

To display the 35mm slide boundary lines:

1. From the **File** menu, choose **Preferences**.
2. Select the **Show 35mm Slide Boundary Guides** check box.
3. Click the **OK** button.

   Two 35mm Slide Boundary Guides appear in the same orientation you have chosen in the Page Setup dialog box. These guides appear in every document.

This preference affects all documents.

Changing Perspectives

You can use a close-up view of objects in your reaction scheme to make sure they are properly positioned. At times, you may want to reduce your view so that you can move groups of objects around the page. You can change the magnification to perform these functions by using the Magnify and Reduce commands in the View menu, the Zoom tool, or the magnification controls.

Magnifying with the View Menu

When you use the View menu to magnify or reduce, the magnification is set to the next higher or lower value. You can magnify up to 400% or reduce to 25%.

Magnify

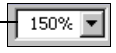
To magnify using the View menu:

1. Select the object around which you want to magnify your view.

   NOTE: If you do not select an object, the last object drawn is the center point of the magnification.

2. From the **View** menu, choose **Magnify**.

   The magnification occurs around the center of the selected object. The magnification percentage appears in the Magnification drop-down list.

Windows  *Macintosh*

You can continue to magnify your view to a maximum of 400%.

Actual Size

To return to the actual size from any other magnification:

- From the **View** menu, choose **Actual Size**.

  The view is returned to the original size.

Reduce

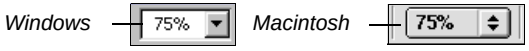
To reduce the magnification:

1. Select an object around which you want to reduce the magnification.

   NOTE: If you do not select an object, the last object drawn is the center point of the magnification.

2. From the **View** menu, choose **Reduce**.

   The reduction in magnification appears in the Magnification drop-down list.



You can reduce the magnification until the entire page fits on the screen. In the reduced view, you can continue to use all of the drawing tools. In particular, you can use a selection tool to rearrange the drawing in order to take better advantage of the space available.

Fit to Window

Fit to Window reduces the magnification until the entire page is visible in the document window.

To view the entire drawing area in a document window at once:

- From the **View** menu, choose **Fit to Window**.

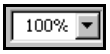
  The Magnification control shows the reduction in magnification that was required to have the entire page appear on the screen.

Using the Magnification Control

When you use the Magnification control, you can display magnifications from 10% to 999% of the normal size of your page. The magnification control allows you to select a specific value.

To use the Magnification controls:

Windows:

- Select a value from the drop-down list 

or type a value.

Macintosh:

Do one of the following:

- Select a value from the drop-down list

.
- Select **Other** from the drop-down list. In the dialog box that appears, type a value and click **OK**.

Arranging Objects

This section describes methods for positioning, aligning, and layering objects in a document window.

Using Rulers

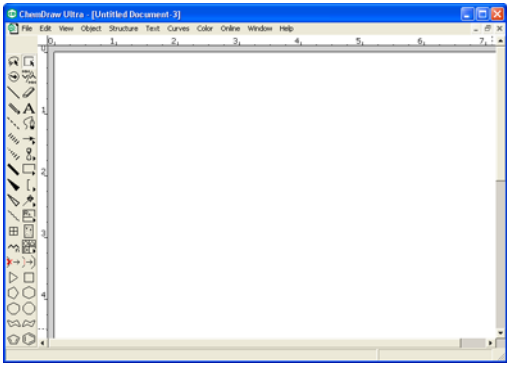
You can use the rulers to position objects a measured distance away from some reference point or create objects of an approximate size. The units used for the ruler are set in the Preferences dialog box, where you have the choice of inches, centimeters or points.

Showing Rulers

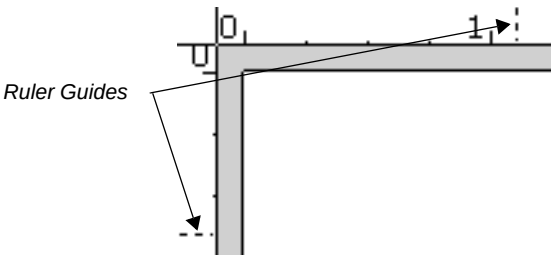
To display the rulers:

- From the **View** menu, choose **Show Rulers**.

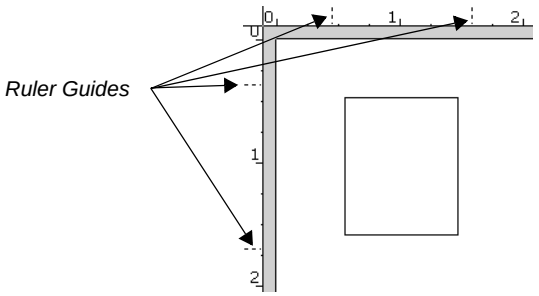
A check mark appears next to the Show Rulers command, and the rulers appear along the top and left edges of a document window.



As you move the pointer, Ruler Guides appear on each ruler, indicating the position of the pointer.



Ruler guides also appear when you drag selected objects. In this case, however, there are two Ruler guides that bracket the object. With this bracketing you can quickly establish the height and width of the selected objects.



Hiding Rulers

To Hide the rulers:

- From the **View** menu, choose **Show Rulers**.

  The check mark disappears.

Using the Crosshair

Use the Crosshair to align objects relative to each other, and to space objects a consistent distance apart. The axes of the Crosshair can be moved within a document window.

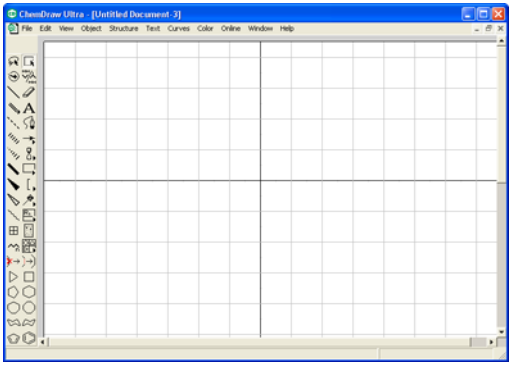
Displaying the Crosshair

To show the Crosshair:

- From the **View** menu, choose **Show Crosshair**.

  A check mark appears next to the Show Crosshair command and the Crosshair appear within a document window.

To assist you in aligning objects, the Crosshair includes grid lines that extend from the major division marks on each axis.



You can also show the Rulers while the Crosshair are displayed so that you can see the unit measurement associated with each of the divisions on the Crosshair axes.

Moving the Crosshair

To move the Crosshair:

1. Position the pointer where the Crosshair axes intersect.

   When the pointer is near to the center of the Crosshair, it changes to an arrow.
2. Drag the **Crosshair**.

To constrain the movement of the Crosshair to the X- or Y-direction:

- Shift+drag the crosshair.

Aligning Objects using the Crosshair

To use the Crosshair to align objects do one of the following:

- Move the Crosshair axes and align it with the object.
- Select an object and drag it until it is aligned with either axis of the Crosshair, or a grid line.

In either case, if a bond or side of the object is parallel to one of the axis, it disappears when it is exactly positioned over a Crosshair axis.

To align another object on the Crosshair:

1. Select a second object.
2. Drag the second object to the Crosshair axis or grid line and align it to the first.

You can also move selected objects in small increments to align them with the Crosshair using the Arrow keys available on some keyboards:

To move 1 point in the direction of an Arrow key:

NOTE: *1 point equals 1/72 inch or 0.035 cm.*

- Select the objects and then press an **Arrow** key.

To move 10 points using the Arrow key, for example, to the right:

- Press **Alt+Right Arrow** or **Option+Right Arrow**.

Hiding the Crosshair

To hide the Crosshair:

- From the **View** menu, choose **Show Crosshair**.

  The check mark next to the Show Crosshair command disappears.

Centering on a Page

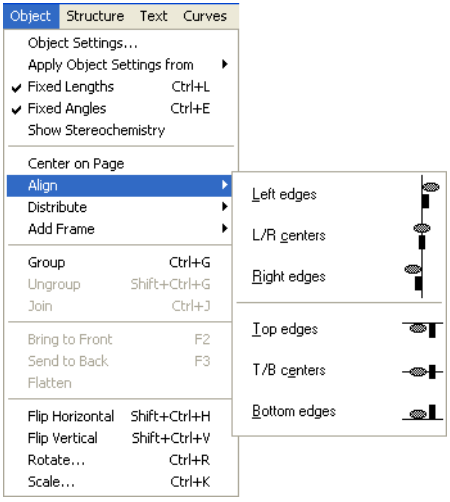
To center an object (or group of objects) at the center of the page:

1. Select the object you want to center using a selection tool.
2. From the **Object** menu, choose **Center on Page**.

   The selected objects move so that the center of the Selection rectangle is positioned at the center of the page.

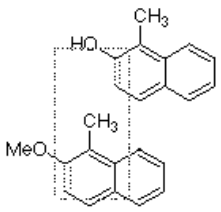
Aligning Objects

Use the Align commands to align objects relative to each other. Examples of the types of alignments are shown on the menu.

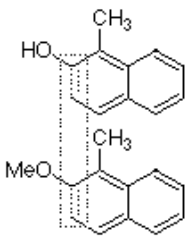


To align two or more objects:

1. Select the objects with a selection tool.



2. From the **Align** submenu, choose one of the Align commands.



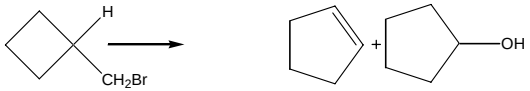
If you select only part of a structure or group with a selection tool, only that part is used for the alignment operation, but the entire structure or group is moved.

Distributing Objects

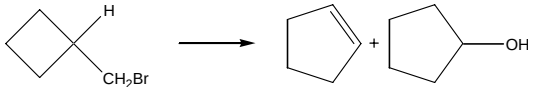
Use the distribute commands to distribute objects horizontally or vertically and at an equal distance apart. For reactants and products with different shapes, select the parts of the objects to distribute.

To distribute 3 or more objects:

1. Select the 3 or more objects to distribute.



2. On the **Object** menu, point to **Distribute**, and then choose **Vertically** or **Horizontally**.



The space between the objects is equalized. The upper, lower, right, and left positions of objects in your selection remain unchanged.

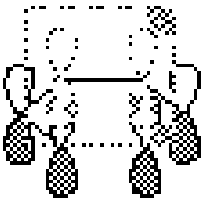
Front to Back Ordering

The front to back ordering is a useful method for changing the orientation of one object relative to another object within the same picture layer. For additional information specific to the layering of bonds, see "Changing Bond Crossings" on page 71.

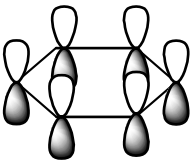
Send to Back

To place one object behind another within a layer:

1. Select the object that you want to send to the back, in this example, the two upper orbitals.



2. From the **Object** menu, choose **Send to Back**.



The selected object appears behind all other objects in the same layer.

Bring to Front

To place one object in front of another within a layer:

1. Select the object that you want to move forward.
2. From the **Object** menu, choose **Bring to Front**.

   The selected object now appears in front of all other objects.

NOTE: *When bonds have 3D coordinates, those coordinates always determine the visible bond crossings. Bring To Front and Send To Back have no visible effect in this case.*

Creating Tables

You can create tables of ChemDraw objects with the Table tool or tables of text with the Text tool.

Creating Tables with the Table Tool

Tables created with the Table tool are containers for drawings and data. To place a structure in a table, you can draw it directly in the table, or copy or drag it into the table.

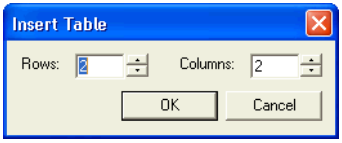
The Table tool enables you to do the following:

- Create and modify tables
- Customize the borders
- Add or delete rows and columns
- Resize the table and its cells manually
- Fit a cell around its contents automatically
- Align cell contents

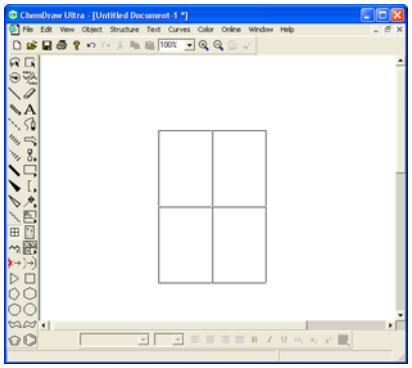
To create a table with the Table tool:

1. On the **Main Tools** palette, click the **Table** tool .
2. Do one of the following:
   - Click and drag in the document window to create the table.

     The default table has two rows and two columns.
   - Click in the document window, type the numbers of rows and columns in the Insert Table dialog box, and then click **OK**.



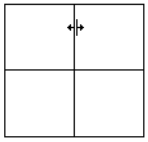
The table appears in the document window.



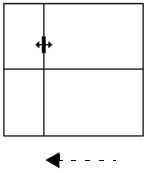
To resize the rows or columns:

1. Place your pointer on the border to resize.

   The pointer changes to a double-headed arrow.



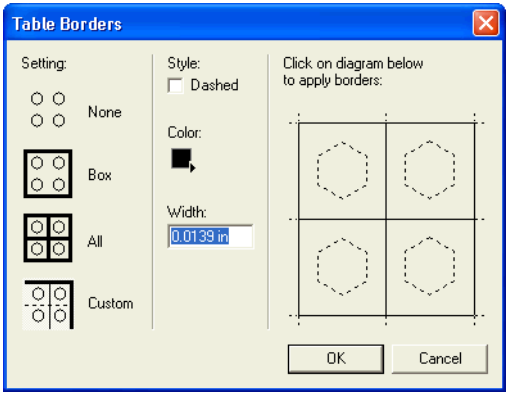
2. Drag the border to the desired size.



To customize the borders of the table:

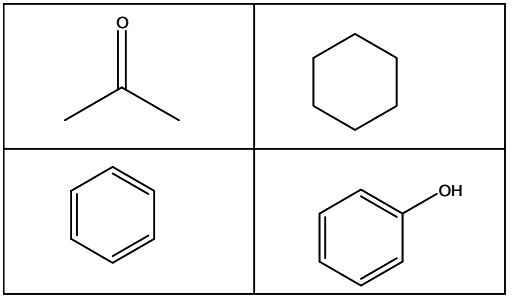
1. With the Table tool selected, point to a border and right-click or option-click.

   The Table Borders dialog box appears.



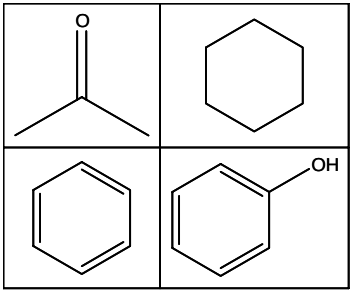
2. In the Setting section, click the borders to which you want to apply the settings.
3. In the Style section, select the style, color and width of the border to apply.
4. In the table diagram, click the borders to customize.
5. Click **OK**.

To make a cell fit around its contents, such as in the table shown below:



1. Point to a border and right-click.
2. Choose **Size To Fit Contents**.

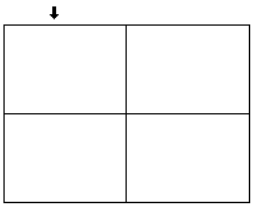
The cells resize to fit around the contents.



To add rows or columns to the table:

1. Point to the border where you want to add the rows or columns.

   The arrow appears as shown below.



2. Right-click or Option-click and from the menu that appears, choose the appropriate option:

If you want to ...	Then choose ...
add an empty row above the indicated row	**Add Row Before**.
add an empty row below the indicated row	**Add Row After**.
add an empty column to the left of the indicated column	**Add Column Before**.
add an empty column to the right of the indicated column	**Add Column After**.
delete the indicated row and its contents	**Delete Row**.
delete the indicated column and its contents	**Delete Column**.

To align all of the objects in the table:

- Point to a border, right-click, point to **Align**, and then choose the alignment you want.

  The cell contents shift and stay in a fixed position relative to the cell. The default alignment is unaligned.

Creating Tables with the Text Tool

ChemDraw allows you to create tables of text using the Tab key with the Text tool.

Creating the First Row (column headings)

To create the first row and establish the columns of a table:

Click the **Text** tool.

3. Click in a document window where you want the table to start.
4. Type a caption.
5. Press **Tab**.

   A second caption box appears.
6. Type a second caption.

   The second column is placed 20 points (20/72 inch, 0.71 cm) to the right of the first.

7. Press **Tab** again to create a third column, and so on.

NOTE: *The style, font, and size that you set in each column are maintained in all the rows that follow.*

The following illustration shows the creation of new columns using the Tab key.

Compound	M.W.	LogP	LD50
	tab	tab	tab

To change the spacing between columns one point at a time while editing a caption:

Select the caption.

8. Move the caption with the arrow keys.

   For more information on moving objects, see "Moving Objects" on page 111.

To create another column with this same spacing as the previous:

- Press **Tab**.

  A third caption text box appears.

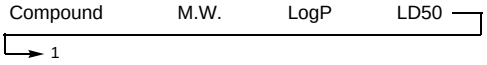
Creating a New Row

To start a new row that is exactly aligned with the first:

- Press Tab twice at the end of a row.

  A caption text box appears exactly aligned under the first caption positioned exactly 20 points below the first caption in the first row.

The following diagram illustrates the creation of a new row.



To change the spacing between rows as you create the table:

Select the captions in a row.

9. Move the captions using the arrow keys.

   For more information on moving objects, see "Moving Objects" on page 111.

To continue and fill in the row with captions:

- Press **Tab** to create another caption in the row, and then press **Tab** twice to begin a new row.

  The spacing between the newest row and the row directly before it have the same spacing that you specified between the previous two rows.

Adjusting Row or Column Spacing

To use a selection tool to adjust the spacing in a table:

Select all of the captions with a selection tool.

10. Shift+drag the caption.

The movement is constrained to the X-axis or Y-axis so that you can maintain the row or column alignment.

Moving Around In Tables

To move within an existing table:

Click the **Text** tool and select a caption.

11. Press **Ctrl+arrow** or **Command+arrow** to move to the next caption in the direction of the arrow.

Alternatively, you can use the following key combinations:

Use ...	**To move ...**
Tab	right
Shift+Tab	left
Ctrl+Enter or Command+Return	down

Use ...	To move ...
Ctrl+Shift+Enter or Command+Shift+Return	up

Inserting a New Row

To insert a row:

Select a selection tool and select a row of captions.

12. **Shift+drag** the selected row.

    Shift constrains the movement to the Y-axis to maintain the column alignment.

13. Select the first caption in the row above or below the space you created.

14. **Ctrl+Shift+drag** or **Command+Shift+drag** to create a copy of the caption and position it in the empty space you created.

    The placement of this copied caption sets the position of the inserted row.

To fill in the inserted row with caption text:

Click the **Text** tool and select the first caption in the inserted row.

15. Type new text.

16. Press **Tab** to move to the second caption in the inserted row, and so on.

Chapter 12: Sharing Information

Overview

ChemDraw includes many of the standard system commands for transferring information within and between ChemDraw documents, and between ChemDraw and documents created using other applications.

You can transfer information using:

- the Clipboard
- drag and drop
- file formats

When you drag-and-drop ChemDraw information, or use the clipboard, the object you are copying can be edited.

Using the Clipboard

You can use the clipboard to transfer part or all of the information within an active document window between applications on the same computer or a networked computer. Use the standard "Copy-and-Paste" or "Cut-and-Paste" tools to transfer information to any application that supports these tools. The information is transferred as a ChemDraw drawing object. Double-clicking on it will open ChemDraw and allow you to edit the object. See "Embedding Objects (Windows)" on page 194 and "Edit Graphic Object (Macintosh)" on page 195 for more information on editing ChemDraw objects embedded in other documents.

If the Clipboard contains ChemDraw structures and you are pasting into another ChemDraw document, the pasted information is scaled to the settings in the current document. For more information, see "Autoscaling" on page 193.

If you are pasting the ChemDraw drawing into a document from which you are planning to print to a PostScript printer, see"Transferring PostScript (Macintosh)" on page 195.

SMILES and SMIRKS Strings

A SMILES string is a way to describe a chemical structure in a line of text. Several software packages use SMILES strings as a way to enter and store chemical structure information.

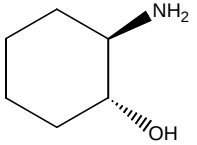
A SMIRKS string is a way to describe chemical reactions in text. If you select a reaction and use the Copy As SMILES command, a SMIRKS string is copied to the clipboard. If you use the Paste Special SMILES command when a SMIRKS string is on the clipboard, a reaction is pasted into your document.

Creating SMILES Strings

To create the SMILES string for the following structure:

1. Select the structure using a selection tool.
2. From the Edit menu, point to **Copy As**, and then choose **SMILES**.

   The SMILES string corresponding to the trans-2-amino-cyclohexanol molecule is transferred to the Clipboard.



N[C@@H]1[C@H](O)CCCC1

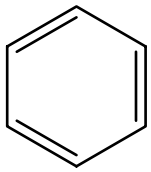
To display the SMILES string:

- Paste the string in a document window.

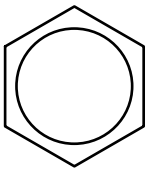
When the SMILES string is on the Clipboard, you can transfer it to another application that can interpret and manipulate SMILES strings.

If you select more than one structure in ChemDraw, and choose Copy SMILES from the Edit menu, the SMILES string for each structure is copied to the Clipboard and separated from the previous SMILES string by a period.

SMILES supports an alternate notation for aromatic structures using lowercase letters. ChemDraw generates this type of SMILES string for any structure drawn with explicit aromatic bonds, either by using the Aromatic bond type in the Atom Properties dialog box, or by placing a circle within any ring structure.



C1=CC=CC=C1



c1ccccc1

Pro Pasting SMILES from Clipboard

If you have a SMILES string, then you can automatically convert that text string into a ChemDraw structure.

To paste a SMILES string as a ChemDraw structure:

1. Select the SMILES string using the Text tool.
2. From the Edit menu, choose **Copy**.
3. From the Edit menu, point to **Paste Special**, and then choose **SMILES**.

The SMILES string is drawn as a structure.

NOTE: *Pasting SMILES uses the same routines as the Structure CleanUp command. For more information, see "Using Variable Attachment Positions" on page 127.*

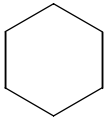
Pro Creating SLN Strings

You can copy a ChemDraw structure to the Clipboard as an SLN string for export to a Tripos application.

To copy a ChemDraw structure as an SLN string:

1. Select a structure.
2. From the Edit menu, point to **Copy As**, and then choose **SLN**.

   The Structure is copied to the clipboard as an SLN String.



C[1]CCCCC@1

Using Drag-and-Drop

You can use the drag-and-drop feature to copy objects to place in other documents. To use this feature in other applications, they must support drag-and-drop. As when using the clipboard, the information is transferred as a ChemDraw object and can be edited.

You can also use the drag-and-drop feature to create clipping files (Macintosh) or scrap files (Windows).

To create a clipping file or a scrap file:

1. Select an object in a ChemDraw document.
2. Drag the selection out of the ChemDraw document window onto the desktop.

A clipping file or a scrap file is created on your desktop.

To view the information within a clipping file or a scrap file:

- Double-click the file's icon.

  A window appears showing the ChemDraw drawing. Click the close box to close the clipping file's window.

To use the contents of a clipping or scrap file in a document:

- Drag the clipping or scrap file into an open window of an application that supports the drag-and-drop feature.

  The contents of the clipping or scrap file are copied to the open window. The clipping or scrap file is unchanged.

Transferring Between ChemDraw Documents

Whether you use the clipboard or drag-and-drop, when you move objects into another ChemDraw document they will behave in a well-defined way. In particular, you should be aware of the behavior of:

- Autoscaling
- Bonds
- Atom Labels
- Captions
- Non-bond Objects and Color
- Pasting to an Empty Document Window

Autoscaling

When you transfer ChemDraw objects using the Clipboard or drag and drop from one ChemDraw document (the source document) to another ChemDraw document (the destination document), the objects are automatically scaled to match the document settings of the destination document. Automatic scaling assures that the objects being transferred match the settings of the current document.

Bonds

All bonds drawn in the source document using the values specified in the Drawing Settings dialog box can be changed to use the Drawing Settings in the destination document.

Any resized bond in the source document is scaled in the destination document. The scale factor is based on the ratio of the bond's length after resizing (source) to the Fixed Length in the Drawing Settings dialog box (source). This scaling process maintains the source document proportions in the destination document. All values in the Drawing Settings dialog box are scaled using this method.

For example, the Fixed Length is set to 1.0 cm in a source document. A benzene ring is resized in to 200%. The bond length is then 2.0 cm: a ratio of 2.0 cm:1.0 cm or a scale factor of 2. In the destination document, the Fixed Length set to 1.7 cm. When the benzene ring is pasted into the destination document, the bonds are scaled by a factor of 2 to a final bond length of 3.4 cm.

Atom Labels

Atom labels are scaled the same way as bonds.

For example, in the source document, the atom label font size is set to 16 points. One or two atom labels in the source document are resized to 8 points, a ratio of 8:16 or a scale factor of 0.5. The destination document has an atom label font size is set to 14 points. When the atom label is pasted into the destination document, the font size is scaled by a factor of 0.5 to give a final atom label font size of 7 points.

Captions

ChemDraw autoscales captions are autoscaled using the ratio of the fixed length in the destination document to the fixed length in the source document times the caption font size. The font size of the caption can be any size and is not related to the setting in the Settings dialog box. This assures that captions are always in proportion to the bonds with which they are pasted.

For example, If the source document has a fixed length of 1.0 cm and the destination document has a fixed length of 2.0 cm, and the caption you are pasting is 12 points, then the resulting caption size after autoscaling is (2.0 cm /1.0 cm) x 12 points = 24 points.

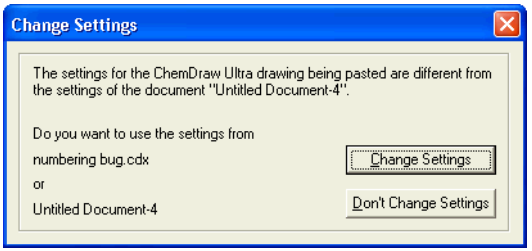
Non-bond Objects and Color

All objects that are not affected by settings in the Document Settings dialog boxes, such as arrows and boxes, are scaled to maintain the same proportions to bonds that were present in the source document.

With the exception of the foreground and background color, the other colors present in the selection to be pasted are added to the destination document's Color Palette if they are not already present (up to a maximum of 20 total colors). The background color in the destination document is unchanged, and all objects colored using the foreground color are changed to match the foreground color in the destination document.

Pasting to an Empty Document Window

If you paste a ChemDraw drawing into an empty ChemDraw document and the settings between the documents are different, the Change Settings dialog box appears:


Change Settings
The settings for the ChemDraw Ultra drawing being pasted are different from the settings of the document "Untitled Document-4".
Do you want to use the settings from
numbering bug.cdx
or
Untitled Document-4
Change Settings
Don't Change Settings

To change the settings in the destination document to match the settings in the source document:

- Click **Change Settings**.

  All of the settings in the destination document are changed to match those of the source document. All of the colors in the Color Palette of the destination document are changed to those specified in the source document.

To scale the objects from the source document to the settings in the destination document:

- Click **Don't Change Settings**.

  The settings from the source document are scaled to those in the destination document using the ratios given above.

NOTE: *If the source document was created in a ChemDraw version earlier than 3.0, the name of the document appears as "Unknown" in the dialog box.*

Embedding Objects (Windows)

ChemDraw supports the Object Linking and Embedding (OLE) protocol on Windows. This allows you to edit ChemDraw structures that are

pasted in other types of documents. ChemDraw is an OLE server, which means it can create OLE objects that can be copied and pasted into other OLE client applications.

When a drawing is transferred from ChemDraw into another document type that supports OLE, you can open the drawing and edit it from within the client application.

For example, to edit a ChemDraw drawing inserted into Microsoft Word for Windows version 6.0 or later, do one of the following:

- Select a ChemDraw drawing in a Word document and from the Edit menu, point to **CS ChemDraw Drawing Object**, and then choose **Edit**.
- Double-click a ChemDraw drawing in a Word document.

  The ChemDraw tools and menus replace those of Word. Use the ChemDraw tools to edit the drawing.

When you have finished making changes:

- Click in another area of the document.

  The Word tools and menus are restored.

Edit Graphic Object (Macintosh)

ChemDraw supports the Edit Graphic Object (EGO) protocol for editing ChemDraw structures pasted into other types of documents. When you drag an object from ChemDraw into another type of document that supports the EGO protocol, or copy it with the clipboard, you can double-click on the object and it appears in a ChemDraw document window. When you close the ChemDraw document window, any changes you made are reflected in the other document.

NOTE: *As of this writing, versions of Microsoft Word after 5.0 do not support EGO.*

Transferring PostScript (Macintosh)

To obtain the highest quality drawings possible on a PostScript printer, ChemDraw creates both a screen representation and a PostScript representation of your drawing. PostScript is a page-definition language used to describe drawings. Many printers, including most Apple LaserWriter printers, use PostScript to create high quality output.

For best print quality under all circumstances, we recommend that you leave the Include PostScript and Include ChemDraw Laser Prep preferences selected (default) when you copy and paste from ChemDraw to other applications. The ChemDraw Laser Prep option adds approximately 11K to 12K to each drawing, but these options give you the greatest flexibility if you give your document to someone else or later want to print it on a PostScript printer.

If you never plan to print to a PostScript printer or never plan to give your document to someone who uses a PostScript printer, you can turn the preferences off.

To deselect the PostScript preferences:

1. From the File menu, choose **Preferences**.
2. Deselect **Include PostScript** and **Include ChemDraw LaserPrep**.

To transfer only a few drawings to another document:

NOTE: *You can also transfer drawings to a document in a remote location whose printer cannot be initialized by ChemDraw.*

- In the Preferences dialog box, select **Include PostScript** and **Include ChemDraw Laser Prep**.

The PostScript commands and the ChemDraw Laser Prep are transferred with each drawing. The transferred drawings can be printed independently of ChemDraw.

If you do not check the Include PostScript check box when printing to a PostScript printer ChemDraw sends QuickDraw commands to the printer. For more information, see "Printing Background Color" on page 28.

To print to a non-PostScript printer:

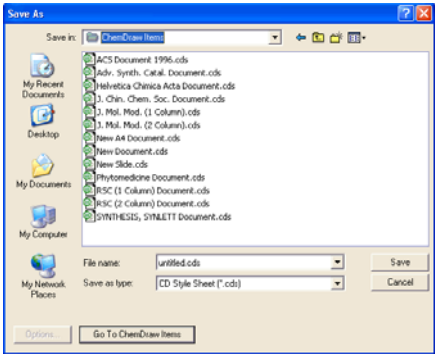
- Deselect both **Include PostScript** and **Include ChemDraw Laser Prep** on the General tab of the Preferences dialog box.

Importing and Exporting

Many applications can use the information contained within a ChemDraw document and saved to another file format. Similarly, ChemDraw can import and work with information in a number of file formats. Not all formats are supported for both import and export. See the individual format descriptions for details. File formats are available in a pop-up menu at the bottom of the "Open" and "Save As" dialog boxes.

To export a file:

1. From the File menu, choose **Save As**.



2. In the Save As dialog box, do the following:
   a. Type a name for the file and choose a location in which to save it. Use the "Go To ChemDraw Items" button to quickly locate the ChemDraw Items folder.
   b. Select a file format from the bottom of the dialog box.
   c. Click **OK** or **Save**.

   A copy of the current document is saved in the format you specified. The current document remains unchanged.

Some file formats do not support atom labels that contain nicknames or structural fragments. When you save in these formats, ChemDraw automatically expands all atom labels and saves the file using the expanded form. For more information, see "Expanding Labels" on page 125.

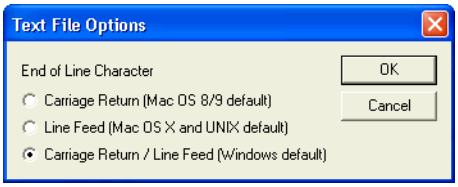
The following formats do not support nicknames or structural fragments:

- Connection Table
- MSI MolFile
- SMD

Some formats can be saved with different options. If a format has no save options, the "Options" button is grayed out. The following text-based formats can use the Text Options:

- ChemDraw XML
- CML
- Connection Table
- ISIS/TGF
- ISIS/Reactions
- MDL MolFile
- Molecular Simulations MolFile

- SMD


Text File Options
End of Line Character
OK
Cancel
Carriage Return (Mac OS 8/9 default)
Line Feed (Mac OS X and UNIX default)
Carriage Return / Line Feed (Windows default)

Other format options are noted in format descriptions.

Graphics export border preference

An explicit preference option allows the user to specify the size of the border when exporting pictures. This preference affects the output of all graphical formats, including but not necessarily limited to: wmf, pict, eps, tiff, gif, bmp, and png. It applies to both the clipboard and saved files.

The default value is 2 points (0.278 in; 0.071 cm). The value can be zero, meaning that the exported image is exactly snug against the objects in the graphic. However, this is not recommended because a bug in Windows causes clipping at the edges of metafiles when they are reduced in size. The default value should prevent clipping with reductions to about 20% of original size.

File Formats

ChemDraw supports both import and export (except as noted below) of the following file formats. To export a ChemDraw file to one of these formats, use the **Save As...** option when saving. For additional information on importing files, see "Inserting Objects from Other Applications" on page 204.

Format	Import	Export
Bitmap (*.bmp)	YES	YES
ChemDraw Template (*.ctp, *.ctr)	YES	YES
ChemDraw (*.cdx)	YES	YES
ChemDraw XML (*.xml)	YES	YES
ChemDraw 3.5 (*.chm)	YES	YES
ChemDraw 2.0 and ChemDraw 2.1 (*.chm)	YES	NO
ChemDraw Stationery/Style Sheet (*.cds)	YES	YES
Connection Table (*.ct)	YES	YES
Chemical Markup Language (*.cml)	YES	YES
Encapsulated PostScript (Macintosh) PostScript (*.eps) (Windows)	YES	YES
Graphic Image Format (*.gif)	YES	YES
ISIS (*.skc, *.tgf, *.rxn)	YES	YES[a]
JCAMP (*.jdx, *.dx)	YES	NO
JPEG (*.jpg, *.jpeg)	YES	NO
MDL MolFile (*.mol)	YES	YES

Format	Import	Export
MDL RGFile (*.rgf)	YES	YES
Molecular Simulations MolFile (*.msm)	YES	YES
PICT (Macintosh)		
Portable Network Graphics (*.png)	YES	YES
Standard Molecular Data (*.smd)	YES	YES
Galactic Industries (.*spc)	YES	NO
Template Style Sheet (*.cts)		
Windows Metafile (*.emf, *.wmf)	YES	YES
TIFF file (*.tif)	YES	YES

[a.] May have limitations. See the appropriate section in the text.

Bitmap (.bmp)

Bitmap (.bmp) files store raster graphics in an array of individual bits. Bitmap images are the most common format for continuous-tone images. Because they represent a fixed number of pixels, bitmaps are resolution dependent and may appear jagged and lose detail if they are scaled on-screen or printed on a higher resolution printer than they were created for.

ChemDraw Template (*.ctp, *.ctr)

Use the ChemDraw Template file format to save template documents that appear in the template pop-up menu.

ChemDraw (*.cdx)

The ChemDraw file format is the native format for ChemDraw version 4.0 and later. This is a public tagged file format that stores information about a ChemDraw structure in a series of data blocks. This format is designed to be easily generated and interpreted by other programs. This format accurately stores anything that can be drawn in ChemDraw.

NOTE: *Imported drawings saved within a ChemDraw file created using ChemDraw for Macintosh are lost when the file is opened using ChemDraw for Windows. The same applies for objects saved in ChemDraw for Windows and opened on a Macintosh. However, all ChemDraw specific information is preserved.*
Imported drawings include any graphics pasted into a ChemDraw document from another Macintosh application. They also include Chem3D drawings imported using the Insert Object dialog box or the "Get 3D Model" Edit menu command in ChemDraw for Windows.

ChemDraw XML (*.xml)

The cdxml file format is an interpreted version of cdx that conforms to the XML specification unlike binary cdx format. cdxml is text-based but contains some data. For information about XML in general, see www.xml.org.

ChemDraw 3.5 (*.chm)

ChemDraw 3.5 file formats are used for saving or opening ChemDraw documents using the version 3.5.x of ChemDraw. These documents can also be

opened in versions 3.0, 3.0.1, 3.0.2, and 3.1 of ChemDraw as long as atom properties are not used in the files.

NOTE: *When you save a ChemDraw file in one of these formats, all features specific to later versions are lost. For example, multi-attached atom labels, variable attachment points, and multicenter bonds are not be saved.*

ChemDraw 2.0 and ChemDraw 2.1 (*.chm) Import Only

ChemDraw 2.0 and ChemDraw 2.1 file formats are used for opening ChemDraw documents using the version 2.x file format of ChemDraw for Macintosh. You cannot save files in these formats.

ChemDraw Stationery/Style Sheet (*.cds)

Use ChemDraw Stationery file format to save document settings and other objects.

Pro Connection Table (*.ct)

The Connection Table file format is a simple format that saves a list of atom connectivities in terms of an element, serial number, X and Y coordinates, bond order, and bond type. For more information, see , “Chemistry File Formats” on page 267

Pro Chemical Markup Language (*.cml)

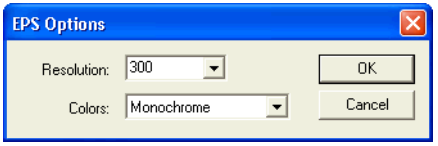
CML is an extensible, chemically-aware markup language based on XML. ChemDraw supports both import and export of the format. More information can be found at http://www.xml-cml.org/ and http://cml.sourceforge.net.

Encapsulated PostScript (Macintosh) PostScript, *.eps (Windows)

Encapsulated PostScript (EPS) files are ASCII text files containing the scalable PostScript representation of a ChemDraw drawing that can be opened using other applications and platforms. There are two types: one containing text only, and one containing a graphic representation of the drawing. The latter are known as Postscript with Preview or Postscript Mac. For text only files, programs that do not support the display of raw PostScript can only print, not view an image on screen.

Use EPS files to share ChemDraw drawings with desktop publishing applications such as Adobe PageMaker and QuarkXPress.

The “Options” dialog box allows you to select the resolution (in dpi) and color depth of the saved file The defaults are 300 dpi and Monochrome. For Windows EPS with Preview, there is also a Preview option (default: WMF).



If you select a color option, all colors are saved in the EPS file except for the Background color. To save an EPS file with a colored background, create a large colored rectangular box using the Drawing Elements tool and choose Send to Back before saving the file. For more information, see “Drawing Boxes” on page 100 and “Using Multi-Center Bonds” on page 126. These options only affect embedded images. Objects created in ChemDraw always output at maximum resolution and in full color.

To include correct PostScript font names in Windows EPS files, you must have Adobe Type Manager (ATM) installed. Only ATM fonts are saved in the EPS file.

Resolution

Available resolutions range from 72 (computer monitor) to 1440 dpi (high resolution output). When choosing a resolution, keep in mind that the size of the file increases as the square of the resolution.

Color

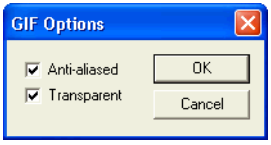
You can select from the following color options:

- **Monochrome**—Forces all objects to black and white.
- **Grayscale**—Translates colors to shades of gray.
- **24-bit RGB** —Stores colors using computer monitor style of color encoding.
- **32-bit CMYK**—Uses printing press style of color encoding. Groups each color type sequentially. This provides better compression.

GIF Image (*.gif)

Graphics interface format (GIF) is useful for working with the hypertext markup language (HTML) used in displaying information on the World Wide Web. A GIF image can be displayed directly on a Web page rather than having to download the drawing for viewing in a Helper application.

The default GIF format conforms to the GIF 89a specifications with transparent backgrounds. You can change this from the options menu.



Pro ISIS/SKC and ISIS/TGF

You can save a ChemDraw document in an ISIS file format for export to an ISIS application, or import a file created by an ISIS application into ChemDraw.

ChemDraw Pro provides two ISIS file formats:

- **ISIS/Sketch** (*.skc)—For saving files as a binary sketch file for transfer to another ISIS application running on the same operating system (this format is used on the Clipboard).
- **ISIS/TGF** (*.tgf)—For saving as an ASCII text file (a Transportable Graphics File) for transfer to ISIS applications on different platforms.

NOTE: *When transferring between ChemDraw and ISIS/Draw, if information in a file or on the Clipboard contains only non-bond, unsupported objects, the information is imported as a WMF (metafile) or PICT graphic. However, if a supported object, such as a bond, is also in the file or on the Clipboard, then only the supported object appears.*

NOTE: *Object types in ISIS not supported in ChemDraw, such as polymers, are not transferred. Object types in ChemDraw not supported in ISIS are not transferred. However, in some cases, such as different arrow types, the arrow is converted to the most similar form.*

Pro ISIS/Reactions (*.rxn)

The ISIS/Reactions format is an MDL-developed format for storing chemical reaction information used by the ISIS family of products and others.

For single step single or multi-line reactions, ChemDraw uses the point of the reaction arrow as the dividing line to determine which molecules in a reaction are reactants and which are products.

NOTE: *You cannot save a reaction with an intermediate step accurately in the RXN file format.*

Molecules whose centers are behind or above the tip of the arrow are considered reactants, and all remaining molecules are products. The reaction arrow can be at any orientation; it does not have to be parallel to the x-axis. If a reaction contains multiple arrows, then the largest arrow is used as the reaction arrow.

Reaction mapping and reaction center information is stored in the rxn output file.

Pro JDX (*.jdx, *.dx) Import Only

The Joint Commission on Atomic and Molecular Properties (JCAMP) developed the JDX file format for spectral data. JDX is a public, but not well defined format that has numerous variations. ChemDraw supports many of the more common spectral variations with uniform x-axis spacing.

ChemDraw also supports Bruker NMR JCAMP data, which is saved with a .dx file extension

When you import JDX files, they appear in the window with a spectrum of a standard size that can be re-sized by dragging.

You can export spectral data as part of a .cdx file only.

JPEG (*.jpg, *.jpeg) Import Only

ChemDraw supports import of digital images compressed with the widely used JPEG (Joint Photographic Experts Group) algorithm. JPEG images are imported as objects, and can be scaled after importing.

Pro MDL MolFile (*.mol)

MDL Information Systems, Inc. MolFile (MDL MolFile) file format is used by several other Windows, Macintosh, and UNIX chemical databases and drawing applications such as ISIS/Draw™, ISIS/Base™, MACCS™, and REACCS™.

ChemDraw Pro provides two MDL MolFile formats:

- MDL MolFile (Text)
- MDL MolFile (Mac) for Macintosh only. This file type is saved with an mMol file type and can be saved and opened with ISIS.

MDL MolFile files are ASCII text files that can be created or edited in common word processing applications or text editors. Atom and bond property information is stored in the MolFile.

MDL RGFile (*.rgf) file format is used by several other chemical databases and drawing applications. The MDL File RGFile supports alternate groups whereas an MDL Molfile cannot. When you save a ChemDraw file that contains alternate groups as an MDL MolFile, it is automatically saved as an MDL RGFile.

Pro Molecular Simulations MolFile (*.msm)

Molecular Simulations MolFile format is an ASCII text file used by applications such as ChemNote™. You can save a ChemDraw Pro document in Molecular Simulations MolFile format for export to one of these applications.

NOTE: *ChemDraw uses the file extension ".msm" for Molecular Simulations MolFiles rather than the standard ".mol", used by Molecular Simulation, Inc. ChemDraw recognizes files with the ".mol" file extension as MDL MolFiles. In addition, the extension ".msi" used in earlier*

versions of ChemDraw is no longer recognized in ChemDraw. To open Molecular Simulations MolFiles that have a ".mol" or ".msi" extension you must first change the extension to ".msm".

PICT (Macintosh)

PICT files contain a QuickDraw representation of a ChemDraw drawing that can be used by various drawing applications. You can save a ChemDraw document in the PICT format so it can be opened by one of these other applications. The PICT file format contains ChemDraw structural information. PICT files created by earlier versions of ChemDraw can be reopened and edited by ChemDraw version 8.0. However, the pictures contained in PICT files created by versions of CS ChemDraw earlier than version 3.5, or by other applications, are treated as a single, non-editable, imported picture.

All colors are saved in the PICT file except for the Background color.

PICT scaled 4X (Macintosh)

PICT scaled 4X files are the same as PICT files, except that the drawing is four times larger. When these larger files are placed into certain other applications and shrunk back down to 1/4 size, they may provide higher quality output than regular PICT files.

PNG file (*.png)

PNG (Portable Network Graphics) format is an alternative to the GIF format for adding graphics to web pages. You can save, but not open, files in PNG format. The PNG format is fairly new and was designed to address many of the shortcomings of the GIF format. In particular, the PNG file format offers true color images, is less prone to transmission errors and offers a full alpha channel for specifying background or transparency options.

For additional information about PNG visit: http://www.boutell.com/boutell/png/

Pro SMD (*.smd)

Standard Molecular Data (SMD) file format, version 4.3, is an ASCII text file commonly used by programs that search Chemical Abstracts Databases such as STN Express™. You can save your ChemDraw document in SMD format and use the file for searching in a Chemical Abstracts database.

Pro SPC (.*spc) Import Only

The SPC file format was developed by Galactic Industries as part of the GRAMS software, which reads spectral data from every type of spectrometer and converts them to SPC format. SPC is a well-defined, proprietary, but open standard format for spectral data.

ChemDraw imports most one-dimensional spectral spc formats. When you import an SPC file, it appears in the window with a spectrum of a standard size that can be re-sized by dragging.

You can export spectral data as part of a .cdx file only.

Pro Template Style Sheet (*.cts)

The Template Style Sheet file format is used for saving document settings and row and column characteristics for creating ChemDraw Template documents.

Windows Metafile (*.wmf)

The Windows Metafile file format saves the Graphic Device Interface (GDI) representation of a ChemDraw drawing. Using the WMF file format you can transfer ChemDraw drawings to other applications, such as Microsoft® Word, that support that WMF file format on the same or

different computers rather than using the Clipboard. The WMF file format contains ChemDraw structural information.

TIFF file (*.tif)

TIFF format (Tagged Image File Format) is a high resolution format commonly used for saving graphics for importing into desktop publishing applications on the same or on different computer platforms. TIFF images can be saved using a variety of resolution, color, and compression options. As TIFF images can get rather large, choosing appropriate options is important. The TIFF format is for export only.

Resolution

Available resolutions range from 72 (computer monitor) to 1440 dpi (high resolution output). When choosing a resolution, keep in mind that the size of the file increases as the square of the resolution.

Color

You can select from the following color options:

- **Monochrome**—Forces all objects to black and white.
- **RGB Indexed**—Stores colors using computer monitor style of color encoding.
- **CMYK Planar**—Uses printing press style of color encoding. Groups each color type sequentially. This provides better compression. For example: CCCCCC-MMMMMMYYYYYYKKKKK rather than CMYKCMYKCMYKCMYK. This option produces far better compression than using the PackBits compression method. However, many desktop publishing packages do not support CMYK Planar files.
- **CMYK Contiguous**—Uses printing press style of color encoding. Stores colors non-sequentially. For example: CMYKCMYK. The PackBits compression type provides no compression for this type of file.

NOTE: *If objects in your document are black and white they are saved black and white regardless of which Color options you set. If you import drawings from other applications and want them to print Black and White you must set the Color option to Monochrome.*

Compression

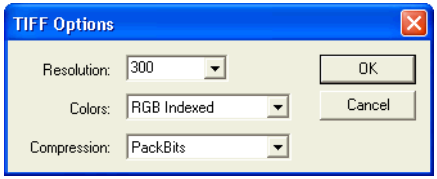
You can select from the following compression options:

- **PackBits**—Used to reduce files size by encoding repeating bytes of information as output when using the CMYK Planar color option. Below is a highly simplified representation of this compression scheme. For a line of color information such as: CCCCC-MMMMMYYYYYKKKKK, the compression yields a smaller file by representing the information as C46M5Y5K.
- **CCITT Group 3**—Used for fax transmissions of images.
- **CCITT Group 4**—Used for fax transmissions of images.
- **Deflate**—Similar to LZW compression. Works well with all Color and Resolution options.

Setting TIFF options

To set these options:

- Click the **Options** button in the Save dialog box to display the TIFF options dialog box.



3. Select the options you want and click **OK**.

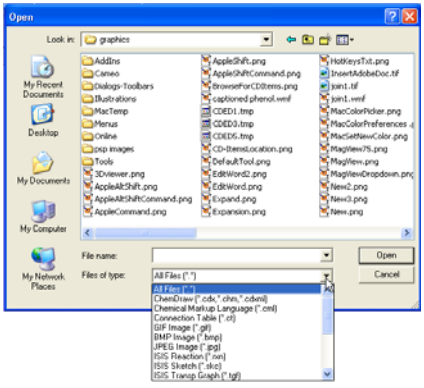
NOTE: *In the Macintosh version you may want to increase the memory allocated to ChemDraw if you are saving large TIFF files.*

Inserting Objects from Other Applications

You can insert graphics or documents created in other applications into ChemDraw. You can edit inserted objects using the ChemDraw Edit menu. Inserted objects can be resized or rotated using the resize and rotate handles of a selected object. You cannot flip inserted objects.

To insert a graphic from another application into ChemDraw:

1. From the **Edit** menu, choose**Insert File**.
2. In the Open dialog box, select the file type from the drop down menu.



3. Select the graphic and click **Open**.

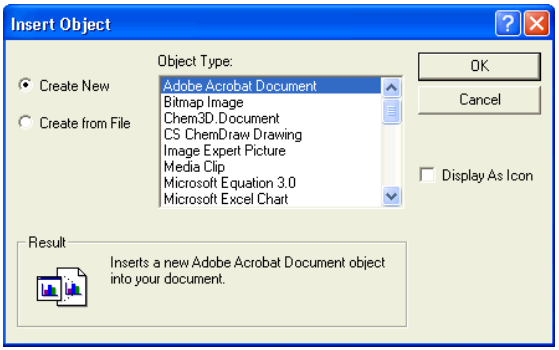
   The file is embedded into the ChemDraw file.

NOTE: *If you select file type "All files" and choose a file type that ChemDraw does not support (such as .txt) you will get an error message, and the file will not be embedded.*

(**Windows only**)
To insert an object from another application into ChemDraw:

1. From the Edit menu, choose **Insert Object**.

   The Insert Object dialog box appears.



2. Take the appropriate action:

If you want to ...	Then ...
create a new object	a. Click **Create New**. b. Select the **Object Type**. c. Click **OK**.
insert an existing graphic	a. Click **Create from File**. b. Type the path or browse to the object to insert. c. Click **OK**.

Transferring ChemDraw Documents Across Platforms

Use the following procedures to transfer ChemDraw documents across platforms. From the following table, determine the versions of the ChemDraw software between which you want to transfer documents and then follow the appropriate instructions.

When you transfer ChemDraw files across platforms, fonts are not transferred. If a font in the transferred document is not available, ChemDraw substitutes fonts for those that are available on the new platform.

Transferring from Macintosh to Windows

To be able to open a ChemDraw file created on the Macintosh in Windows, follow the instructions for the appropriate versions shown in the table below.

From Mac Version	To Windows Version	Instructions
≥ 4.0	≥ 4.0	Save as ChemDraw and add .cdx to the file name.
≥ 4.0	3.x	Save as ChemDraw 3.x and add .chm to the file name.
≤ 3.5.x	= 3.x	Save as ChemDraw and add .chm to the file name.

Transferring from Windows to Macintosh

To be able to open a ChemDraw file created in Windows on the Macintosh, follow the instructions for the appropriate versions shown in the table below.

From Windows Version	To Mac Version	Instructions
≥ 4.0	≥ 4.0	Save as the default ChemDraw (.cdx).
≤ 3.5.x	≥ 4.0	Save as ChemDraw 3.x (.chm).
≤ 3.5x	≤ 3.x	Save as ChemDraw 3.x (.chm) and follow the instructions in "Transferring files to ChemDraw/Plus 3.1 for the Macintosh" below.

Transferring Files to ChemDraw/Plus 3.1 for the Macintosh

Use the following procedure to transfer a ChemDraw for Windows file to ChemDraw/Plus 3.1 for the Macintosh. A file translator such as PC Exchange or Apple File Exchange must be running on your Macintosh.

To transfer from Windows to ChemDraw/Plus 3.1 for the Macintosh:

1. In ChemDraw for Windows, save the file in the **ChemDraw (.chm)** format.
2. Insert the disk with the ChemDraw for Windows files into the Mac floppy drive.
3. If you are using PC Exchange, double click the floppy disk icon to display the files.

4. From the **Control Panels**, select **PC Exchange**.
5. Select **Add**.
6. Change the DOS suffix to **.chm**.
7. In the application selection, find **CSC Chem-Draw** on your Mac and click once to highlight the selection.
8. Change the document type to **CHMS**.

If you are using a translator other than PC Exchange, you need to use an editor such as ResEdit or Disktop to change the type and creator of the files being transferred. The type should be "CHMS" and the creator should be "CHMD."

Chapter 13: ChemDraw/Excel

The ChemDraw/Excel add-in is an extension of Microsoft© Excel© for Windows. ChemDraw/Excel enables you to:

- Add chemical structures and other data from ChemDraw or a ChemFinder database to an Excel spreadsheet.
- Search using the same search features as ChemFinder.
- Perform calculations on chemical structures.

See the ChemOffice manual for information on other CambridgeSoft add-ins for Excel.

NOTE: Any commands you use operate on the cells, not the pictures in the cells.

Setting Up ChemDraw/Excel

When you install *ChemFinder*, ChemDraw/Excel is automatically installed. Before you use ChemDraw/Excel for the first time, do the following:

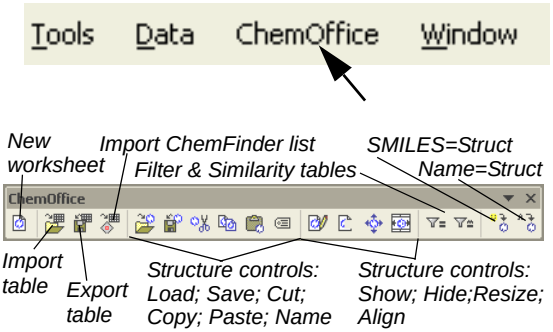
1. From the **Tools** menu, select **Add-Ins**.

   The **Add-Ins** dialog box appears.

2. In the **Add-Ins** dialog box check the **ChemDraw for Excel** checkbox and click **OK**.

   A ChemOffice worksheet appears. When a ChemOffice worksheet is active, ChemDraw/Excel appears in the title bar and the ChemDraw tool bar is active.

   A ChemOffice menu is added to the Excel menu bar and a ChemOffice tool bar appears.



3. From the **Tools** menu, point to **Macro** and select **Security**.

   The **Macro Security** dialog box appears.

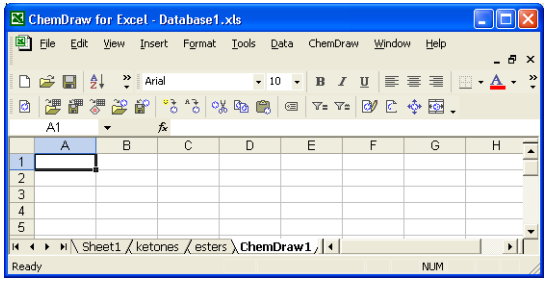
4. In the **Macro Security** dialog box click the **Security Level** tab and set the security level to **Medium**.

   NOTE: ChemDraw/Excel no longer requires this step. You must set security to Medium only if you will be using ChemDraw/Excel worksheets from version 8 or earlier without conversion.

5. Click **OK** to save and exit.

To create a ChemOffice worksheet:

- From the **ChemOffice** menu, select **New ChemOffice Worksheet**, or click .



Importing Tables

ChemDraw/Excel allows you to import from the following sources:

- **MDL SDFiles**—Imports all records in the file. Each structure is given the name stored in the SDFile.
- **ChemDraw databases** —Imports all fields stored in the main form. Molecular weight and formula fields are not imported because ChemDraw/Excel calculates them. Each structure is named Structure <*n*>, where *n* is a unique number.

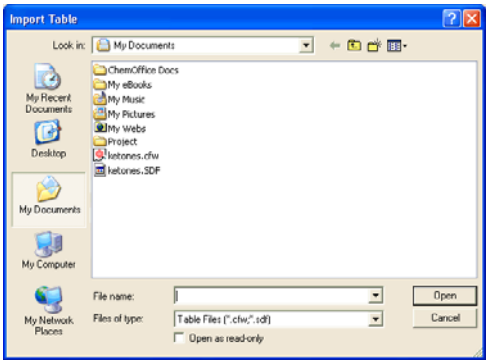
NOTE: In order to import .cfw files into Excel, make sure you save them with the "allow CAL/OLE Automation access" security setting checked. See "Setting Security Options" in Chapter 3 of the ChemFinder manual for details.

When you import a table, structure data are transformed into structure drawings in the first column, and all other fields are imported in separate columns.

To import a table:

1. Select the cell where you want the import to start. The upper left corner of the import is at this cell. Data is filled down and to the right.
2. From the **ChemOffice** menu, select **Import Table** or click .

   The Import Table dialog box appears.



3. Type or select the file name to import and click **Open**.

   All records are added to your spreadsheet.

Converting and Upgrading

Instead of copying and pasting information from a non-ChemDraw/Excel worksheet, you can convert the existing worksheet into a ChemDraw/Excel worksheet.

To convert a worksheet:

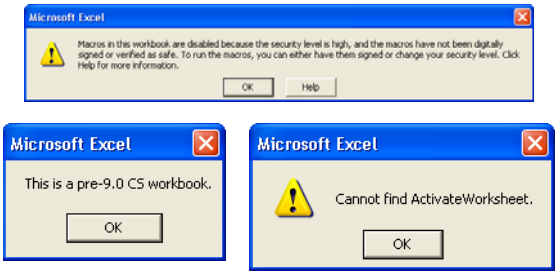
- Select **Convert Worksheet** from the **ChemOffice** menu.

  The work sheet is converted to a ChemDraw/Excel worksheet.

Upgrading Workbooks

ChemDraw/Excel 9.0 improvements have made workbooks created with older versions incompatible. You can open and maintain old workbook for-

mats, but you may get error messages (depending on your Excel security settings) and will be asked if you want to upgrade each time you open them.


Microsoft Excel
Macros in this workbook are disabled because the security level is high, and the macros have not been digitally signed or verified as safe. To run the macros, you can either have them signed or change your security level. Click Help for more information.
OK
Help
Microsoft Excel
This is a pre-9.0 CS workbook.
OK
Microsoft Excel
Cannot find ActivateWorksheet.
OK

To upgrade a workbook:

1. From the **Tools** menu, point to **Macro** and select **Security**.
2. Click the **Trusted Sources** tab and make sure that CambridgeSoft Corporation is listed as a trusted source. Make sure the **Trust access to Visual Basic Project** checkbox is selected.
3. Select **Upgrade Workbook** from the **ChemOffice** menu.
4. To maintain tight security, go back to the **Macro Security** dialog box and uncheck the **Trust access to Visual Basic Project** checkbox.

Importing Hit Lists

You can perform a search in ChemFinder and then import the hit list structures with data into Excel using the Get ChemFinder List command.

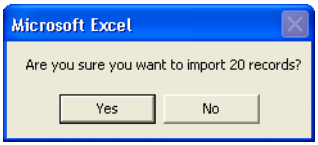
To use the Get ChemFinder List command, ChemFinder must be open with a hitlist present.

Importing a Hitlist

To import a hitlist:

1. From the **ChemOffice** menu, select **Get ChemFinder List**, or click the icon.

   A message box similar to the one below appears appears:

2. Click **Yes** to import the hitlist.

   The records are imported into Excel, starting with the currently selected cell and moving down and to the right.

Error Messages

If all conditions required to use the Get ChemFinder List command are not met, one of the following error messages may appear.

ChemFinder is not running, would you like to start it up?

ChemFinder is not running. Do the following:

1. Click **Yes**.

   The message "After loading your desired database and performing your search, return to Excel and redo the operation." appears.

2. Click **OK**.

   ChemFinder opens.

3. Open a database and perform a search.
4. Return to Excel and from the **ChemOffice** menu, select **Get ChemFinder List**, or click .

No database loaded in ChemFinder. Load a database and perform your search. Then return to Excel and redo the operation.

ChemFinder is running, but no database is loaded. Do the following:

1. Click **OK**.

   ChemFinder moves to the front.
2. Open a database and perform a search.
3. Return to Excel and from the **ChemOffice** menu, select **Get ChemFinder List**, or click .

Form has no database or hitlist has no records. Load a database and perform your search. Then return to Excel and redo the operation.

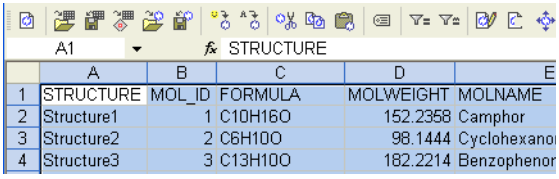
1. Click **OK**.

   ChemFinder moves to the front.
2. Open a database and perform a search.
3. Return to Excel and from the **ChemOffice** menu, select **Get ChemFinder List**, or click .

Exporting Tables

ChemDraw/Excel allows you to export tables to MDL SDFiles.

Selected cells are exported to a specified file. If no cells are selected, the entire spreadsheet is exported. The first column of the area to export must have the word "Structure" in its top cell. Structures outside the first column will be discarded.



	A	B	C	D	E
1	STRUCTURE	MOL_ID	FORMULA	MOLWEIGHT	MOLNAME
2	Structure1	1	C10H16O	152.2358	Camphor
3	Structure2	2	C6H10O	98.1444	Cyclohexano
4	Structure3	3	C13H10O	182.2214	Benzophenor

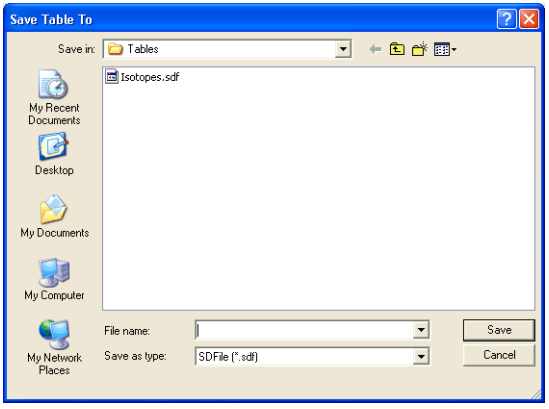
To export data:

1. Select the information to export:

If you want to export	Then
a specified area of your spreadsheet	Select the area to export.
the entire spreadsheet	Do not make any selection.

2. From the **ChemOffice** menu, select **Export Table** or click .

   The **Save Table To** dialog box appears.



3. Type the file name and click **Save**.

   The table is saved to the specified file.

Adding Structures

You can add chemical structures from any file format supported by ChemDraw to a spreadsheet. The names of added structures are retained. If the structure does not have a name, ChemDraw assigns the name: Structure <*n*>, where *n* is a number unique to the worksheet.

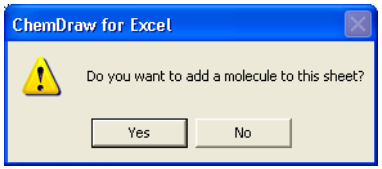
Adding Structures with ChemDraw

The most direct way to insert a new structure into a cell is by using ChemDraw.

To add a structure with ChemDraw:

1. Double-click in a cell.

   The ChemDraw/Excel dialog box appears:



2. Click **Yes**.

   ChemDraw opens.

3. Draw the structure in ChemDraw.

4. From the ChemDraw **File** menu, click **Close and Return to New Molecule**.

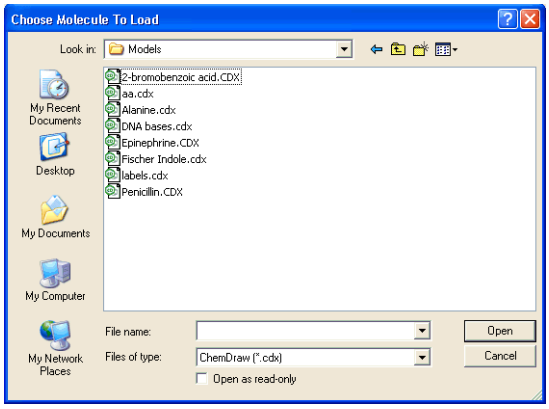
   The new structure appears in the cell.

Adding a Structure From a File

To add a structure from a file:

1. Select the cell into which you want to add the structure.
2. From the **ChemOffice** menu, select **Load Molecule** or click .

   The **Choose Molecule to Load** dialog box appears.



NOTE: You can use the sample molecule file, "SAMPLE.cdx" contained in the ChemDraw system directory, or any .cdx file to load.

3. Type the file name of the structure to add and click **Open**.

   The information is stored in the selected cell.

Adding a Structure with a SMILES String

You can insert SMILES strings into cells and convert them to structures.

To insert SMILES strings:

1. Type or paste SMILES strings into cells.
2. Select the range of cells or single cell to convert.

   NOTE: If you want to keep the original text, copy it and paste it elsewhere.

3. From the **ChemOffice** menu, select **Convert SMILES To Molecule** or click .

If the cell contains a valid SMILES string, it is replaced by a structure. The cell will display a text string starting with "Structure" and followed by a number. To display the structure, click the Show Picture icon.

If the cell did not contain a valid SMILES string, the string remains.

Adding Structures by Name

You can type or paste the names of chemicals into cells and convert them into structures as follows:

1. Enter the names into cells.
2. Select the range of cells to convert.

   NOTE: If you want to keep the original text, copy it and paste it elsewhere. Note that this command can also convert names generated from Excel formulas.

3. From the **ChemOffice** menu, select **Convert Name To Molecule**, or click .

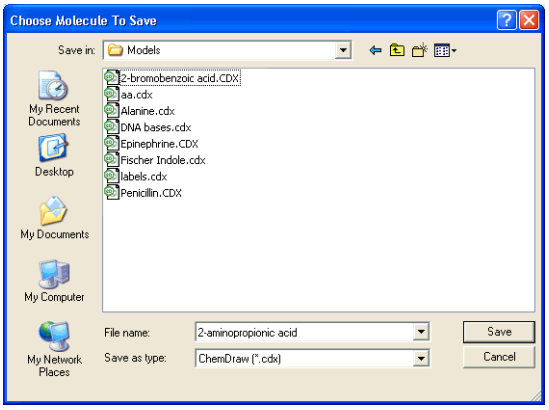
   If the cell contains a name supported by ChemDraw *Name=Struct*, the structure corresponding to that name is added to the cell, with the given name as the name of the cell. To show the structure, select the cell and choose **Show Picture** from the **ChemOffice** menu. For more information about *Name=Struct*, see the ChemDraw User's Guide.

Saving Structures

You can save a chemical structure to a separate file.

1. In the spreadsheet, select the cell containing the structure.
2. From the **ChemOffice** menu, select **Save Molecule** or click .

   The **Save to File** dialog box appears.



3. Select an existing file or enter a new file name, and click **Save**.

   The structure is saved with the name and in the location you selected.

Searching

You can perform the same types of searches in ChemDraw/Excel as you can in *ChemFinder*:

- Exact structure searching
- Substructure searching
- Similarity searching

Filter Tables

Filter tables allows you to search for exact structures and substructures.

To perform a structure search:

1. Select a cell containing the label **Structure**.
2. From the **ChemOffice** menu, select **Filter Table** or click .

   The **Search Query** dialog box appears.

3. Select the search options:

If you want to	Then
search for a structure	a. To load a structure, right-click and select **Read Structure**. b. To edit the structure, double-click it. c. Select the **Search Type**. d. Select the **Filter Type**.
search for a formula	a. Type the molecular formula or formula query in the And/Or Formula Query box. b. select **Clear**.
search for a structure and a formula	a. To edit the structure, double-click it. b. Select the **Search Type**. c. Select the **Filter Type**. d. Type the molecular formula in the And/Or Formula Query box.
see the R-Group Analysis	click the **Show R-Group Analysis** box.
see the previous query	click **Restore Previous Query**.

4. Click **Search**.

   The hit list is displayed in a column named Match. Items matching the search criteria are labeled as TRUE.

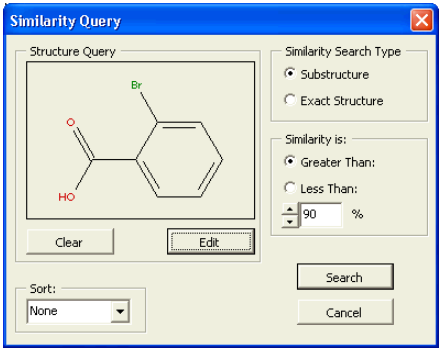
Similarity Searches

You can perform similarity searches to find structures with features corresponding to your search structure. For more information about similarity searching, see the *ChemFinder* User's Guide.

To search for similarity:

1. Select a cell containing the label **Structure**.
2. From the ChemOffice menu, select **Similarity Table** or click .

   The Similarity Query dialog box appears.



3. Select the **Search Type**.
4. Select the **Similarity Is** value.
5. Select the **Sort** order.
6. Click **Search**.

The hit list is displayed in a column named Match. Items matching the search criteria are labeled as TRUE.

Working with Structures

ChemDraw/Excel allows you to rename structures and use the clipboard to cut, copy, and paste structures.

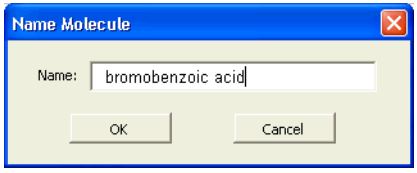
Naming Structures

Excel recognizes certain characters as formulas. To prevent the system from interpreting a chemical structure name as an Excel formula, you can rename a structure.

To name a structure:

1. Select the structure.
2. From the **ChemOffice** menu, select **Name Molecule** or click .

   The **Name Molecule** dialog box appears.



3. Type the name and click **OK**.

Using the Clipboard

You can cut, copy, and paste structures using the clipboard. After you cut or copy a structure, it is placed on the clipboard. You can then paste it into another cell or another application.

To cut a structure from a cell:

1. Select the structure.
2. From the **ChemOffice** menu, select **Cut Molecule** or click .

   The structure is removed from the cell and is placed on the clipboard.

To copy a structure from a cell:

1. Select the structure.
2. From the **ChemOffice** menu, select **Copy Molecule** or click .

   The structure remains in the cell and a copy is placed on the clipboard.

To paste a structure:

1. Select the area into which you want to paste the structure.
2. From the **ChemOffice** menu, select **Paste Molecule** or click .

   The structure is pasted from the clipboard.

Viewing Structures

ChemDraw/Excel allows you to select whether or not to display structures in a cell. You can also adjust the height and width of cells to display their entire contents.

Showing and Hiding Structures

To show structures:

1. Select the cells in which you want to display pictures.
2. From the **ChemOffice** menu, select **Show Picture** or click .

   The structures are displayed in the selected cells.

To hide structures:

1. Select the cells in which you do not want to display pictures.
2. From the **ChemOffice** menu, select **Hide Picture** or click .

   The structures are hidden and the cells resize.

Aligning Structures

A structure may fall outside the boundaries of its cell because it is too big or because it is improperly positioned within the cell. Use the **Align All Pictures** command to enlarge the cell or reposition the structure. If the entire structure is within the cell, regardless of its position, it is not affected by the **Align All Pictures**.

To align structures:

- From the **ChemOffice** menu, select **Align Pictures** or click .

  The cells adjust to display their entire contents.

Resizing Structures

To resize pictures use the **Resize Picture** command.

NOTE: When pictures are resized larger than their cells, use Align Pictures to enlarge the cells. Align Pictures does not make cells smaller.

To resize pictures:

1. Select the chemistry cells whose pictures you want to resize.

   It is not necessary to only select chemistry cells. Non-chemical cells or chemical cells without pictures will be ignored.
2. From the **ChemOffice** menu, select **Resize Picture** or click .

   Resize handles appear on the selected structures.
3. Click-drag the resize handles to resize a picture.

   Any changes you make to a picture is proportionately reflected in the other pictures.
4. To end resizing, click a cell and the pictures are deselected.

Resizing Structures With a Macro

To resize a large number of structures simultaneously, create the following macro:

CFXL.xla!CFxlDoSelectPicture

and assign it to an Excel button or menu item.

Then do the following:

1. Select the cells to be resized.
2. Run the macro.
3. Resize one structure.

   All of the selected structures resize by the same amount.
4. Select the Structure column and align (see "Aligning Structures" on page 215).

For more information on creating and storing macros, see Excel Help.

Using ChemDraw/Excel Functions

ChemDraw/Excel supplies nine functions that return information about chemistry objects in a specified cell. Seven of these functions take only one argument—the cell to which the function refers. The remaining two functions may also take a string as an optional second argument.

The function ISSTRUCTURE is an example of a function that takes only one argument. To determine whether the content of cell A1 in an Excel spreadsheet is a ChemDraw/Excel chemistry object, you type `=ISSTRUCTURE(A1)` into a second cell. The second cell then displays `TRUE` or `FALSE` depending on whether A1 contains a chemistry object.

The function CHEM.COMPOSITION is one of the functions that may take an optional second argument. It works in one of two ways:

With First Argument Only—

Without the second argument, it displays elemental composition by weight percent of the entire chemical structure in cell A1 when you type =CHEM.COMPOSITION(A1) into a second cell. For benzene, it displays C, 92.26; H, 7.74.

With Both Arguments—The second argument lets you find the percent composition of a single element in the structure. Typing =CHEM.COMPOSITION(A1, "C") returns the weight percent of carbon in the structure. For benzene it would display 0.922582. Notice that the display format for a single element is different from that of the whole structure.

The following table outlines the ChemDraw/Excel functions. Only CHEM.COMPOSITION and CHEM.NUM.ATOMS take an optional second argument. The others only take the reference cell argument.

Function	Action
ISSTRUCTURE	Returns TRUE if cell referred to is any ChemDraw/Excel chemistry object including reactions; otherwise it returns FALSE.
ISREACCTION	Returns TRUE if cell reference is any ChemDraw/Excel chemistry object and reaction; otherwise it returns FALSE.
CHEM.FORMULA	Returns formula for structure in cell reference; it returns #N/A error if cell doesn't contain a ChemDraw structure.
CHEM.MOLWEIGHT	Returns molecular weight for structure in cell reference. Returns #N/A error if cell doesn't contain ChemDraw structure.
CHEM.NUM. HBACCEPTORS	Returns number of hydrogen bond acceptors based on topology. Returns #N/A error if cell doesn't contain ChemDraw structure.
CHEM.NUM. HBDONORS	Returns number of hydrogen bond donors based on topology. Returns #N/A error if cell doesn't contain a structure.
CHEM.SMILES	Returns SMILES string for structure. Returns #N/A error if cell doesn't contain ChemDraw structure.

Function	Action
CHEM.COMPOSITION	Returns elemental percent by weight for all elements in structure unless optional second argument specifies a single element symbol as a string. In this case the elemental percent is expressed as a decimal number between 0 and 1. (75.1% would be 0.751) Returns #N/A error if the cell referenced in first argument doesn't contain a ChemDraw structure, or if second argument is not a valid element symbol.
CHEM.NUM.ATOMS	Returns total number of atoms in the structure unless optional second argument specifies a single element symbol as a string. In this case, it returns the number of atoms of that element only. Returns #N/A error if the cell referenced in first argument doesn't contain a ChemDraw structure or if second argument is not a valid element symbol.

Using ChemProp Functions

If you are using ChemDraw Pro or Ultra with the ChemProp add-on installed, you can calculate physical and thermodynamic properties in ChemDraw/Excel. For detailed information on the properties calculated and how ChemProp calculates them, see "Viewing Chemical Properties" on page 141 and Appendix E: "How ChemProp Works."

ChemProp Properties

In ChemDraw/Excel, you can use the ChemProp functions to calculate the following properties:

Property	Function
LogP (Ultra only)	CHEMPROP.LOGP
Molar Refractivity (Ultra only)	CHEMPROP.MR
Henry's Law Constant	CHEMPROP.HENRY.LAW.CONSTANT
Boiling Point	CHEMPROP.BOILING
Freezing Temperature	CHEMPROP.FREEZING
Critical Temperature	CHEMPROP.CRITICAL.TEMP
Critical Pressure	CHEMPROP.CRITICAL.PRESSURE
Critical Volume	CHEMPROP.CRITICAL.VOLUME
Heat of Formation	CHEMPROP.HOF

Property	Function
Gibbs Free Energy	CHEMPROP.GIBBS
Ideal Gas Thermal Capacity	CHEMPROP.IDEAL.GAS
tPSA	CHEMPROP.TPSA

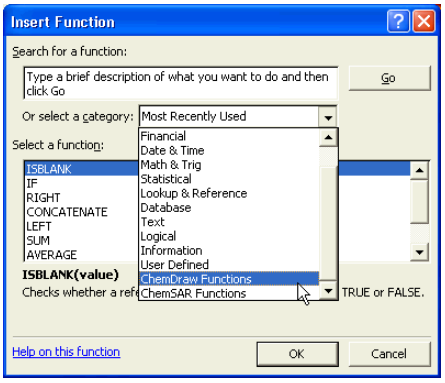
NOTE: Using ChemProp requires that you have a version of ChemDraw that includes ChemProp installed.

Inserting Functions

To insert a ChemDraw/Excel function into your worksheet:

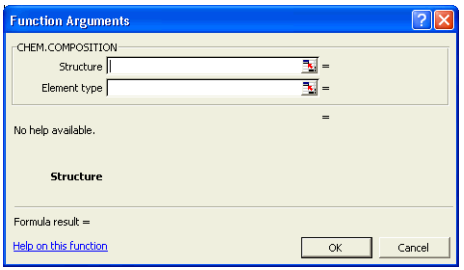
1. Select an empty cell.
2. From the **Insert** menu, select **Function**.

   The **Paste Functions** dialog box appears.
3. Select **ChemDraw Functions**.



4. Select the function to insert from the list and click **OK**.

   A dialog box appears.



5. Enter the structure cell reference for which you want to calculate properties in the **Structure** box.
6. If the function takes a second argument, enter it in the **Element type** box. Element type arguments are optional.
7. Click **OK**.

Each property is calculated using the "best available" method. For more information about calculation methods, see the ChemDraw manual. If the cell reference argument does not point to a valid structure cell, #N/A appears in the cell.

Appendices

This section contains the Appendices for each of the sections.

Section I: General

- Appendix A: Accessing the CambridgeSoft Web Site.
- Appendix B: Technical Support.
  - Contact information and hints on what you should know to effectively report problems. Includes a troubleshooting section.

Section II: ChemDraw

- Appendix C: The Chemistry of ChemDraw.
  - Describes how ChemDraw interprets what you draw and how you can help ChemDraw better interpret what you mean.
- Appendix D: How ChemNMR Works.
  - Describes how ChemNMR estimates chemical shifts for hydrogen or carbon atoms, and it's limitations.
- Appendix E: How ChemProp Works.
  - Describes how ChemProp enables you to calculate predicted values of selected physical and thermodynamic properties.
- Appendix F: Shortcuts and Hotkeys.
  - Contains tables listing ChemDraw shortcuts and hotkeys for both Windows and Mac versions.
- Appendix G: Document Settings.
  - Drawing settings and a sample structure for each of the Style Sheets or Stationery Pads provided with ChemDraw.
- Appendix H: Chemistry File Formats.
  - Most file formats supported by ChemDraw are proprietary or extremely complex and are documented more thoroughly elsewhere. This Appendix describes the connection table format in detail. Note, however, that the format is obsolete, and is documented here for historical purposes only.

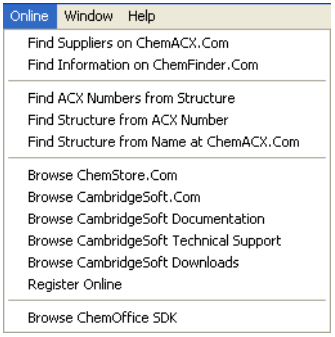
Appendix A: Accessing the CambridgeSoft Web Site

Online Menu Overview

The ChemOffice **Online** menu gives you quick access to the CambridgeSoft web site from within ChemOffice. With the **Online** menu, you can:

- Register your software.
- Search for compounds by name or ACX number and insert the structure in a worksheet
- Use ACX numbers, or names or structures in the worksheet, to search for chemical information
- Browse the CambridgeSoft website for technical support, documentation, software updates, and more

To use the **Online** menu, you must have internet access.



Registering Online

ChemOffice 2005 applications utilize a new security scheme. In order to activate any ChemOffice application, you must register with the CambridgeSoft website to receive a registration code. Upon filling out a registration form, the registration code is sent to you by email. This registration scheme does not apply to site licenses.

If your serial number is invalid for any reason, or if you do not have an internet connection, you will have to contact CambridgeSoft Support to receive a registration code.

You may use your ChemOffice application a limited number of times while waiting for the registration process to be completed. Once the application times out, you must register to activate the software.

In addition to registering your software, you can request literature, or register for limited free access to ChemFinder.com, ChemACX.com, ChemClub.com, and the email edition of ChemBioNews from the **Register Online** link of the **Online** menu. This link connects you to the Cambridgesoft Professional Services page. From this page you can link to a registration form.

To register online:

1. From the **Online** menu, choose **Register Online**.

   The Cambridgesoft Professional Services page opens in your browser.

2. Select the **Register** tab.

Accessing the Online ChemDraw User's Guide

The **Online** menu link **Browse CS ChemDraw Documentation** opens the Cambridgesoft Desktop Manuals page, where you can access current and previous versions of the ChemOffice User's Guide.

To access the CambridgeSoft Manuals page:

1. From the **Online** menu, choose **Browse CS ChemDraw Documentation**.

   The Desktop Manuals page appears. PDF versions of the CambridgeSoft manuals can be accessed from this page.

   NOTE: *If you do not have a CambridgeSoft User account, you will be directed to a sign-up page first.*

2. Click version of the manual to view.

Accessing CambridgeSoft Technical Support

The **Online** menu link **Browse CS ChemOffice Technical Support** also opens the Cambridgesoft Professional Services page. There are a number of links on this page for Troubleshooting, Downloads, Q&A (the ChemOffice FAQ), Contact, and so forth.

Finding Information on ChemFinder.com

The **Find Information on ChemFinder.com** menu item links your browser to the ChemFinder database record of the compound you have selected.

ChemFinder is the public-access database on the ChemFinder.com website. It contains physical, regulatory, and reference data for organic and inorganic compounds.

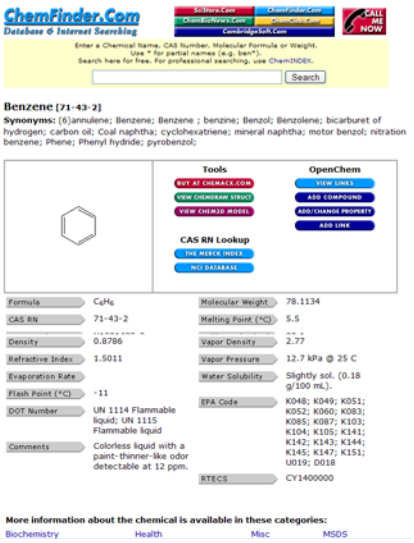
To access ChemFinder.com:

1. In ChemOffice, select a structure you want to look up.
2. From the **Online** menu, choose **Find Information on ChemFinder.com**.

   The ChemFinder.com page opens in your browser with information on the selected structure.

In ChemFinder.com you can search for chemical information by name (including trade names), CAS number, molecular formula, or molecular weight.

Follow the links to do substructure queries.The following illustration shows part of the page for Benzene.



Finding Chemical Suppliers on ACX.com

The **Find Suppliers on ACX.Com** menu item links your browser to the chemacx.com database record of suppliers of the compound you have selected.

ChemACX (Available Chemicals Exchange) is a Webserver application that accesses a database of commercially available chemicals. The database contains catalogs from research and industrial chemical vendors.

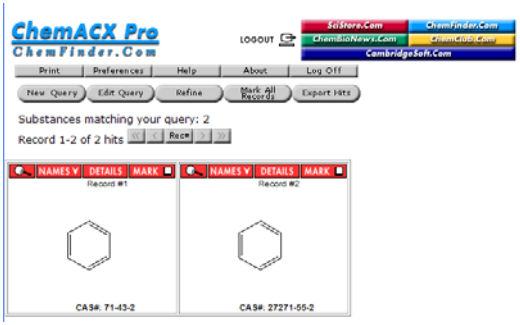
ChemACX allows the user to search for particular chemicals and view a list of vendors providing those chemicals.

To use **Find Suppliers on ACX.Com** menu access:

1. In ChemOffice, select a structure you want to look up.
2. From the **Online** menu, choose **Find Suppliers on ACX.com**.

   The ChemACX.Com page opens in your browser with information on the selected structure.

For example the ChemACX.com page for Benzene is shown below.



For more information on using the ChemACX website, see the ChemOffice Enterprise Workgroup & Databases Manual.

Finding ACX Structures and Numbers

ChemOffice searches ACX and returns information about related structures and numbers. You can place the returned information in your document.

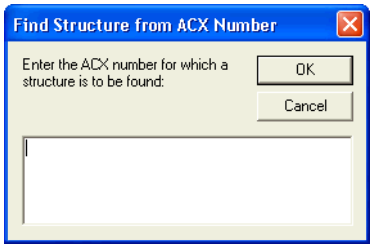
ACX Structures

There are two ways to find ACX structures: by ACX number or by name.

To find a structure that corresponds to an ACX number:

1. From the **Online** menu, choose **Find Structure from ACX Number**.

   The **Find Structure from ACX number** dialog box appears.



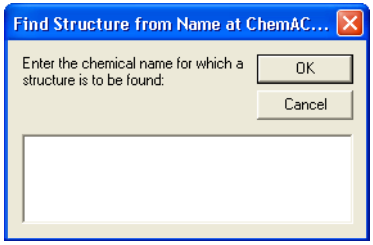
2. Type the ACX registry number.
3. Click **OK**.

   The Structure appears in your document.

To find a structure from a name

1. From the **Online** menu, choose **Find Structure from Name at ChemACX.com**.

   The **Find Structure from Name** dialog box appears.



2. Type in a name. As with ChemFinder.com, you can use a chemical name or a trade name.
3. Click **OK**.

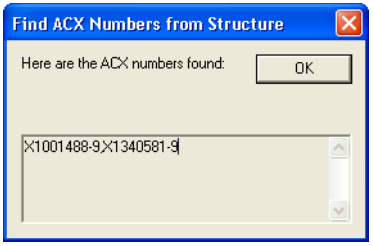
   The Structure appears in your document.

ACX Numbers

To Find an ACX number for a structure:

1. In a ChemOffice document, select the structure for which you want to find an ACX number.
2. From the **Online** menu, choose **Find ACX Numbers from Structure**.

   The ACX number appears in the **Find ACX Numbers from Structure** dialog box.



Browsing SciStore.com

Browse ChemStore.com opens the SciStore (formerly ChemStore) page of the CambridgeSoft web site (http://scistore.cambridgesoft.com/).

To access Browse SciStore.com:

- From the **Online** menu, choose **Browse ChemStore.com**.

  The SciStore.Com page opens in your browser.

You can search SciStore.Com for chemicals, lab supplies, chemistry-related software, and other items you want to buy. You can access ChemACX.Com and other pages from SciStore.Com.

Browsing CambridgeSoft.com

Browse CambridgeSoft.com opens the Home page of the CambridgeSoft web site.

To access the CambridgeSoft Home Page:

- From the **Online** menu, choose **Browse CambridgeSoft.com**.

  The CambridgeSoft web site in your browser.

Check the CambridgeSoft web site for new product information. You can also get to SciStore.Com, ChemBioNews.Com, and other pages through CambridgeSoft.Com.

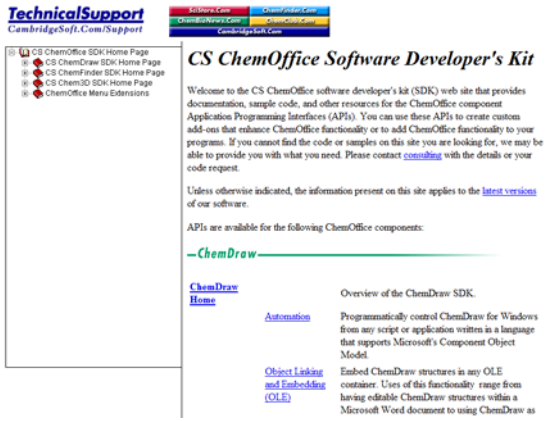
Using the ChemOffice SDK

The ChemOffice Software Developer's Kit (SDK) enables you to customize your applications.

To browse the ChemOffice SDK:

- From the **Online** menu, choose **Browse ChemOffice SDK**.

  The CS ChemOffice SDK page opens in your browser.


TechnicalSupport
CambridgeSoft.Com/Support
SciStore.Com
ChemFinder.Com
ChemBioNews.Com
ChemOffice.Com
CambridgeSoft.Com
CS ChemOffice SDK Home Page
CS ChemDraw SDK Home Page
CS ChemFinder SDK Home Page
CS Chem3D SDK Home Page
ChemOffice Menu Extensions
CS ChemOffice Software Developer's Kit
Welcome to the CS ChemOffice software developer's kit (SDK) web site that provides documentation, sample code, and other resources for the ChemOffice component Application Programming Interfaces (APIs). You can use these APIs to create custom add-ons that enhance ChemOffice functionality or to add ChemOffice functionality to your programs. If you cannot find the code or samples on this site you are looking for, we may be able to provide you with what you need. Please contact consulting with the details or your code request.
Unless otherwise indicated, the information present on this site applies to the latest versions of our software.
APIs are available for the following ChemOffice components:
ChemDraw
ChemDraw Home
Overview of the ChemDraw SDK.
Automation
Programmatically control ChemDraw for Windows from any script or application written in a language that supports Microsoft's Component Object Model.
Object Linking and Embedding (OLE)
Embed ChemDraw structures in any OLE container. Uses of this functionality range from having editable ChemDraw structures within a Microsoft Word document to using ChemDraw as

The ChemOffice SDK page contains documentation, sample code, and other resources for the Application Programming Interfaces (APIs).

NOTE: *You must activate Javascript in your browser in order to use the ChemOffice SDK page.*

Appendix B: Technical Support

Overview

CambridgeSoft Corporation (CS) provides technical support to all registered users of this software through the internet, and through our Technical Support department.

Our Technical Support webpages contain answers to frequently asked questions (FAQs) and general information about our software. You can access our Technical Support page using the following address: http://www.cambridgesoft.com/services/

If you don't find the answers you need on our website, please do the following before contacting Technical Support.

1. Check the ReadMe file for known limitations or conflicts.
2. Check the system requirements for the software at the beginning of this User's Guide.
3. Read the Troubleshooting section of this appendix and follow the possible resolution tactics outlined there.
4. If all your attempts to resolve a problem fail, fill out a copy of the CS Software Problem Report Form at the back of the User's Guide. This form is also available on-line at: http://www.cambridgesoft.com/services/mail
   - Try to reproduce the problem before contacting us. If you can reproduce the problem, please record the exact steps that you took to do so.
   - Record the exact wording of any error messages that appear.
   - Record anything that you have tried to correct the problem.

You can deliver your CS Software Problem Report Form to Technical Support by the following methods:

Internet:
http://www.cambridgesoft.com/services/mail

Email: support@cambridgesoft.com

Fax: 617 588-9360

Mail: CambridgeSoft Corporation

ATTN: Technical Support

100 CambridgePark Drive

Cambridge, MA 02140 USA

Serial Numbers

When contacting Technical Support, you must *always* provide your serial number. This serial number was on the outside of the original application box, and is the number that you entered when you launched your CambridgeSoft application for the first time. If you have thrown away your box and lost your installation instructions, you can find the serial number in the following way:

Macintosh

- With ChemDraw launched, choose **About CS ChemDraw** from the Apple menu. The serial number appears at the bottom left.

Windows

- Choose **About CS <application name>** from the **Help** menu. The serial number appears at the bottom left of the About box.

For more information on obtaining serial numbers and registration codes see:
http://www.cambridgesoft.com/services/codes.cfm

Troubleshooting

This section describes steps you can take that affect the overall performance of CambridgeSoft Desktop Applications, as well as steps to follow if your computer crashes when using a CS software product.

Performance

Below are some ways you can optimize the performance of CambridgeSoft Desktop Applications:

- **Macintosh:** Increase the total amount of memory that the application can use:
  - Select the ChemDraw application icon in the Finder when ChemDraw is not running.
  - From the **Edit** menu, choose **Get Info**. Increase the memory allocation in the Preferred size text box in the Memory Requirements section of the dialog box.
- **Windows:** In the Performance tab in the System control panel, allocate more processor time to the application.
- Install more physical RAM. The more you have, the less ChemOffice Desktop Applications will have to access your hard disk to use Virtual Memory.
- Increase the Virtual Memory (VM). Virtual memory extends RAM by allowing space on your hard disk to be used as RAM. However, the time for swapping between the application and the hard disk is slower than swapping with physical RAM.

  Change the VM as follows:
  - System control panel, Performance tab.

System Crashes

CambridgeSoft Desktop Applications should never crash, but below are the steps you should go through to try to resolve issues that cause computer crashes while using a CS software product.

1. Restart your computer (Macintosh) or restart Windows and try to reproduce the problem. If the problem recurs, continue with the following steps.
2. The most common conflicts concern Video Drivers, Printer Drivers, screen savers, and virus protection. If you do need to contact us, be sure to determine what type and version of drivers you are using.

   Video Driver related problems: If you are having problems with the display of any CambridgeSoft Desktop Application, try switching to the VGA video driver in the display Control Panel (or System Setup, and then retest the problems. If using a different driver helps, your original driver may need to be updated–contact the maker of the driver and obtain the most up-to-date driver. If you still have trouble contact us with the relevant details about the original driver and the resulting problem.

   Printer Driver related problems: Try using a different printer driver. If using a different driver helps, your original driver may need to be updated–contact the maker of the driver and obtain the most up-to-date driver. If you still have trouble contact us with the relevant details about the original driver and the resulting problem.
3. Try reinstalling the software. Before you reinstall, uninstall the software and disable all background applications, including screen savers and virus protection. See the complete uninstall instructions on the CambridgeSoft Technical Support web page.

4. If the problem still occurs, use our contact form at: http://www.cambridgesoft.com/services/mail and provide the details of the problem to Technical Support.

Appendix C: The Chemistry of ChemDraw

Overview

ChemDraw automatically converts lines, characters, and other symbols into chemically meaningful figures as you work. This work occurs in the background, but you can choose to view this chemical data using Check Structure, Analyze Structure, and Expand Atom Labels. ChemDraw also uses this chemical data when exporting to file formats that support only a subset of the notations that ChemDraw does.

This appendix describes how ChemDraw interprets what you draw and how you can help ChemDraw better interpret what you mean.

Chemical Intelligence in ChemDraw

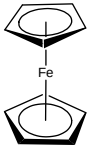
ChemDraw was designed as a tool to aid in chemical communication. Most chemists would understand AcOo-C_6H_4COOH immediately, whether or not they recognized it as aspirin. Most computer programs, however, require what is known as a "complete connection table," in this case, a collection of 21 atoms connected by 5 double bonds and 16 single bonds in a specific pattern. ChemDraw takes what makes sense to a chemist and converts it into what makes sense to another application.

This chemical intelligence can be used as a sophisticated "spelling" checker for chemical compounds. For example, if you're investigating organic acids, a compound with the structural formula CH3COO would probably represent acetic acid. Present the same formula in a paper on transition metal chemistry, and you might be describing a novel methylated cobalt oxide. If you had asked ChemDraw to interpret it beforehand, you would have received a message reporting a valence error, and you might have been prompted either to add a negative charge or to change the capitalization.

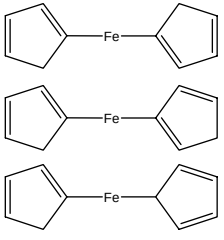
ChemDraw can offer only suggestions. If you and your audience understand what you are trying to depict, then you can ignore these suggestions. In many cases, you can teach ChemDraw to understand the notation you're using. For more information, see "Applying Nicknames" on page 121.

Database Conventions

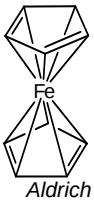
Most databases require not only that you draw a structure in a way that makes sense, but that you draw it in the way that the database expects it. Consider ferrocene, which is represented in at least four different ways in major databases:



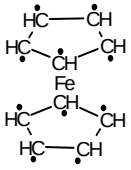
Merck Index



and 3 other isomers
Beilstein



Aldrich



MDL ACD

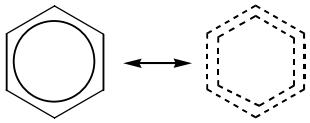
A successful search in one database might not produce any hits in another. When in doubt, consult the documentation for your database, and see if it offers any clues to the conventions used.

Chemical Conventions

The following table describes the chemical conventions understood by ChemDraw.

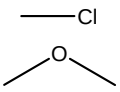
Bond	Description
	Single bond, unspecified stereochemistry.
	Single bond, "down" stereochemistry (into the plane of the paper, away from the viewer), *from* the first drawn atom *to* the second drawn atom.
	Single bond, "up" stereochemistry (out of the plane of the paper, toward the viewer), *from* the first drawn atom *to* the second drawn atom.
	Single bond, mixture of "up" and "down" stereochemistries in some unspecified proportion.
	Dative bond. Often used to indicate polar bonds, such as the N-O bond in pyridine N-oxide.
	Double bond, with *cis*/*trans* stereochemistry as drawn.
	Double bond, with *cis*/*trans* stereochemistry unknown.
	Tautomeric bond, either single or double according to rules of tautomerism.
	Aromatic bond, part of a delocalized resonance system.
	Triple bond.
	Quadruple Bond.

A single bond near a closed circle is recognized as aromatic:

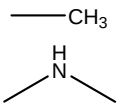


Atom Labels

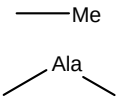
A simple atom label may contain any of the following:



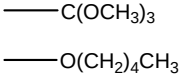
A single element.



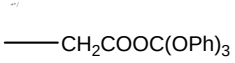
An element and some number of hydrogen atoms.



A nickname.



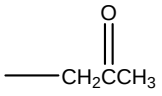
Repeating units within parentheses.



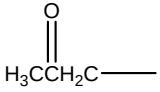
A series of any combination of the above.

When analyzing an atom label, ChemDraw starts at the left and continues to the right, applying standard rules of valence to determine which atoms are bound to which. The exception is with an atom label in Automatic alignment on the left side of a compound. This sort of atom label is displayed "backwards" (H_3CO instead OCH_3) and is therefore parsed from right to left. Standard valences for each atom are defined in the Isotopes Table.

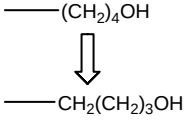
By definition, a "simple" atom label has all bonds attached to the first (or last) character. A multi-attached atom label has bonds connected to more than one character, or has all of its bonds attached to a specific character in the middle of the atom label. Multi-attached atom labels are always parsed from beginning to end, but again the beginning might be on the right if the atom label was in Automatic style and on the left side of the original structure:



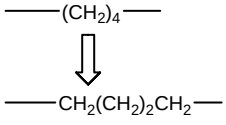
A multi-attached label that is parsed from left to right.



A multi-attached label that is parsed from right to left.



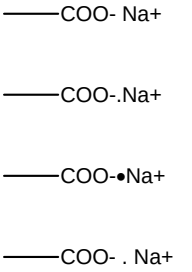
A bond attached to the open parenthesis of a repeating group is treated as if bonded to the first of those groups.



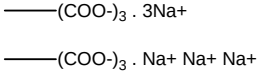
A bond attached to the close parenthesis or repeat count of a repeating group is treated as if bonded to the last of those groups.

Multiple fragments within a single label can be specified in the following ways:

Implicitly, using standard valence rules.



Explicitly, using a space, period (unsuperscripted or unsubscripted), bullet, or combination.



An unsuperscripted, unsubscripted integer at the start of a fragment is recognized as a stoichiometric multiplier and is treated as if the appropriate number of fragments were drawn explicitly.

Chemically Significant Text

Often it is simpler to write a chemical formula like MeOH or H_2O than it is to draw out an entire atoms-and-bonds structure. ChemDraw correctly interprets any *unambiguous* structural formula. For example, $CH_3COCH_2CH_3$ is recognized as methyl ethyl ketone and MeOH is recognized as methanol. On the other hand, C_6H_6 might mean benzene, or it might mean one of over 200 other isomers. C_6H_6

is not recognized by ChemDraw, and generates an error message if you try to analyze it. Generally, empirical formulas (C_2H_6 and H_2SO_4) are not recognized, but structural formulas (CH_3CH_3 and $HOSO_2OH$) are.

Molecular weight and elemental analyses of empirical structures is possible, but the Expand Label command does not work with them. Empirical structures are discarded when they are transferred to other applications that require unambiguous structures.

Chemically-significant text must be entirely in Formula or, for isotopes and charges, Superscript style. ChemDraw does not recognize a chemical formula embedded within a larger block of text.

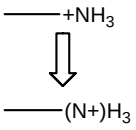
NH_4+ — If you draw a bond, add an atom label, and then delete the bond, you have a chemically meaningful text block whose font, size, and style match other atom labels.

H_2O — If you create a caption with the text tool and set it to Formula style, you have a chemically meaningful text block whose font, size, and style match other captions.

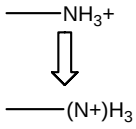
Charges

Charges may be created as part of a textual atom label or with the appropriate symbol from the Chemical Symbols Palette. Charges are always assigned to a specific element in the atom label, whose acceptable valences become those of the similar isoelectronic neutral element.

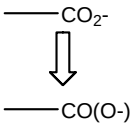
A charge following an element is assigned to that element.



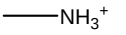
A charge that does not follow an element is assigned to the next element.



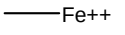
Charges that follow a monovalent element with a repeat count are assigned to the element before that element.



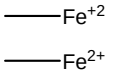
Charges that follow other repeating units are distributed among those units.



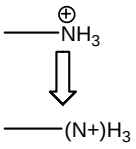
Charges may be superscripted.



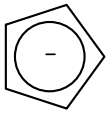
Multiple charges are recognized appropriately.



Charges may have repeat counts as long as both the charge and the repeat count are superscripted.



A "floating" charge placed with the Chemical Symbols Tool is assigned to the nearest atom. If no atom is within the distance set as the Fixed Length, the charge is ignored and not assigned to any atom.

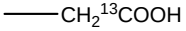


A "floating" charge placed within a delocalized system is recognized by the Analyze Structure function, but is discarded when saved to formats that require all charges to be associated with specific atoms.

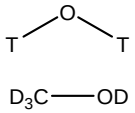
Isotopes and Elements

By default, ChemDraw correctly recognizes all isotopes in the full Table of the Elements. This data is provided by CRC Press, Inc. Isotopes are defined in the Isotopes Table file. You can edit this file to add new isotopes in any text editor.

A superscripted number before the element symbol indicates isotope numbers.



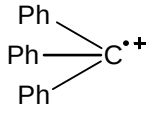
Isotopes can be included anywhere that regular elements can.

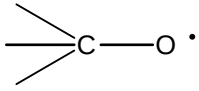


Deuterium and Tritium can be indicated by their one-letter symbols.

Radicals

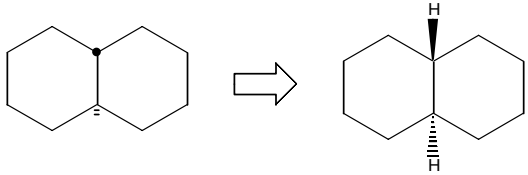
Radicals are indicated with the appropriate symbol from the Chemical Symbols Palette. As with charges, they are assigned to the nearest atom. Radicals always occupy one free valence, in addition to any charge effects.





H-Dot/H-Dash

H-Dot and H-Dash symbols from the Chemical Symbols Palette indicate the stereochemistry of a single hydrogen atom. These symbols are most commonly used in fused systems.



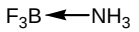
Complexes

Compounds with electron pairs can act as Lewis bases, bonding with Lewis acids that are electron-deficient. Similar behavior can be seen between lone pairs and metals.

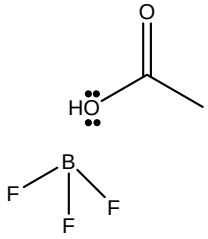
The best representation of these types of interaction is with a dative bond from the electron-pair donor to the acceptor. With a plain bond instead of the dative bond, ChemDraw would report a valence error. The dative bond more accurately represents the electron donation.

Complexes may also be represented with explicit lone pairs and without any bonds.

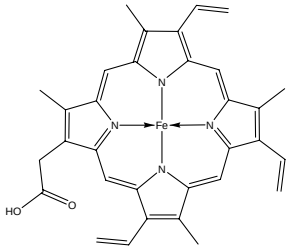
If you use a plain bond to indicate a complex, you may want to set Abnormal Valence to Allowed in the Atom Properties dialog.



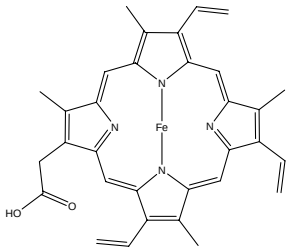
Boron trifluoride-ammonia complex.



Boron trifluoride-acetic acid complex.



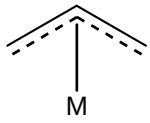
Heme, a compound with two formal covalent bonds and two formal donor-acceptor pairs.



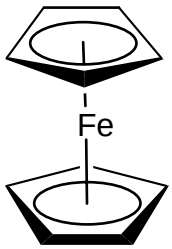
Another representation of heme.

Multi-center Attachments

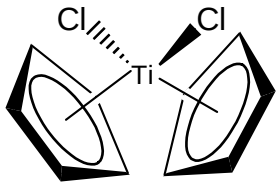
Multi-center attachments are meaningful only when created using Add Multi-Center Attachment from the Structure Menu. This command creates a pseudo-atom that is disregarded during chemical calculations, but still allows you to create diagrams that look meaningful to an experienced chemist.



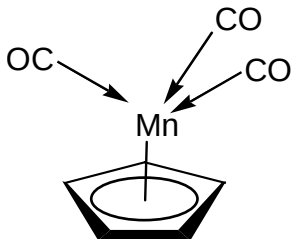
η^3 or π-Allyl complex



Ferrocene, a π-Aryl complex



Cp_2TiCl_2, another π-Aryl complex



η-$C_5H_5Mn(CO)_3$

Stereochemistry

Absolute stereochemistry is calculated for tetrahedral atoms and double bonds according to the Cahn-Ingold-Prelog (CIP) priority rules. The

CIP rules are designed to order ligands by their priority and determine a descriptor based on the orientation of the ordered ligands in space.

A ligand is an entity attached to a stereocenter. For example, a tetrahedral carbon has four ligands corresponding to its four substituents. When a tetrahedral carbon is in a ring, it still has four ligands: the two ligands outside the ring, a third consisting of the ring "unpeeled" clockwise, and a fourth consisting of the ring "unpeeled" counterclockwise.

Five rules are used to determine the priority of ligands are summarized below in simplified form. For more detailed information, see the references. They are checked sequentially as follows:

- **Rule 1**—Higher atomic number precedes lower
- **Rule 2**—Higher atomic mass precedes lower
- **Rule 3**—*cis* precedes *trans*
- **Rule 4**—Like pairs of descriptors precede unlike pairs
- **Rule 5**—R precedes S

ChemDraw checks differences up to 15 atoms distant from the stereocenter.

Stereochemical Indicators

After the ligands are ranked, an indicator is assigned as shown in the following table.[1]

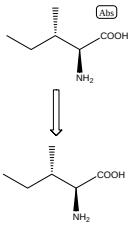
Stereocenter	Indicator
Double bond	Z if the highest ranking ligand of each pair are on the same side of the bond; otherwise E.
Tetrahedral atom	When the lowest-ranking ligand is located behind the central atom: • R when remaining 3 ligands are arranged clockwise in descending order • S when remaining 3 ligands are arranged counterclockwise in descending order • r or s is used for pseudoasymmetric atoms

Stereochemical Flags

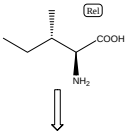
While the chirality of a specific stereocenter can be indicated with the appropriate wedged, hashed, or plain bond, sometimes it is useful to indicate the relative stereochemistry of a molecule as a whole, considering the relationship between all stereocenters. Stereochemical flags apply to the

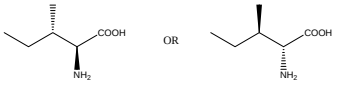
1. R.S. Cahn, C.K. Ingold, and V. Prelog, "Specification of Molecular Chirality", Angew. Chem., Int. Ed. Engl. 1966, 5, 385-414 (errata: 1966, 5, 511); Angew. Chem. 1966, 78, 413-447.
V. Prelog and G. Helmchen, "Basic Principals of the CIP-System and Proposals for a Revision", Angew. Chem. 1982, 94, 614-631; Angew. Chem. Int. Ed. Engl. 1982, 21, 567-583.
P. Mata, A.M. Lobo, C. Marshall, and A.P. Johnson, "The CIP Sequence Rules: Analysis and Proposal for a Revision." Tetrahedron:Asymmetry. 1993, 4, 657-668.

nearest structure; if no structure is within the distance specified by the Fixed Length value, the stereochemical flag is not assigned to any structure.

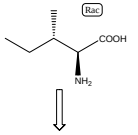


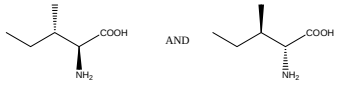
The Absolute flag indicates the exact stereoisomer as drawn.





The Relative flag indicates the exact stereoisomer as drawn, or its enantiomer.





The Racemic flag indicates a mixture of the exact stereoisomer as drawn and its enantiomer.

Polymer Representations

Brackets are used to enclose repeated structures or structural fragments. ChemDraw provides bracket properties to specify the orientation and context of the repeating units. An explanation of the bracket properties is given in "Representing Polymers and Other Repeating Units" on page 163.

References

"Graphic Representations (Chemical Formulae) of Macromolecules (Recommendations 1994)" *Pure Appl. Chem.*, **66**, 2469-2482 (1994).

"Source-Based Nomenclature for Copolymers (Recommendations 1985)" *Pure Appl. Chem.*, **57**, 1427-1440 (1985). Also available at: http://www.iupac.org/publications/books/pbook/
PurpleBook-C7.pdf.

"Basic Definitions of Terms Relating to Polymers (1974)" *Pure Appl. Chem.*, **40**, 479-491 (1974) Also available at: http://www.iupac.org/reports/1996/6812jenkins/
index.html).

Also see the Guide for the authors of papers and reports in polymer science and technology from IUPAC.

Query Properties

By their nature, query properties do not represent actual chemical features, but describe broad classes or groups of features. For information on using query properties, see Chapter 10: Drawing Query Structures.

Analysis Messages

When ChemDraw is unable to analyze your structure fully, two general types of messages are displayed:

- Status messages that report a problem that may not affect the final analysis

- Critical messages that may affect the final analysis

Message	Description
There are too many bonds to this unlabeled Carbon.	Displayed for every unlabeled atom with more than 4 filled valences. Filled valences include sum of bond orders, charge, radicals, and free sites. Aromatic bonds count 1.5 each, rounded down unless it is the only bond to the atom. Charge is signed and includes charge implied by dative bonds. The Substituents query property treats Free Sites, Up to and Exactly the same way: an atom with 2 explicit bonds and "Substituents: Up To 3" or "Substituents: Exactly 3" or "Substituents: Free Sites 1" has three filled valences.
An atom in this label has an invalid valence.	Displayed in a variety of cases where ChemDraw cannot find a place to put a bond or cannot find a bond to put on an atom. Valid valences for each element are listed in the Isotopes Table file.
ChemDraw can't interpret this label.	Displayed when ChemDraw finds text that it cannot identify as an element, nickname, generic nickname, or alternative group name.
Parentheses don't match.	Displayed when parentheses cannot be matched into nested open-close pairs.
This label has conflicting or unassignable charges.	Displayed when a plus and minus charge have been assigned to the same element, charges have been assigned in more than one way, or a charge has been assigned to a nickname, generic nickname, or Alternative Group name.
Formula cannot be computed for queries.	Displayed for every label that contains a generic nickname, an element list or an alternative group. This is a status message only; analysis continues as if the problematic label were not selected.
Text not in Formula style won't be interpreted.	Displayed for the first caption that is not an atom label or Alternative Group name, and which contains any text not in Formula, Subscript, or Superscript style. This is a status message only, and appears only once regardless of how many captions are in the selection.
This named alternative group contains no attachment point.	Displayed for any structure within an Alternative Group Box where the structure lacks an attachment point. This is a status message only.

Message	Description
This named alternative group contains fragments with inconsistent valences.	Displayed for any Alternative Group Box whose contained structures have varying numbers of attachment points. Since all structures within an Alternative Group Box are to be used interchangeably, they must have the same number of attachments. This is a status message only.
This named alternative group contains no fragment.	Displayed for any Alternative Group Box that is empty. This is a status message only.
Part of a molecule is outside of the alternative group definition.	Displayed for any Alternative Group Box whose border crosses part of a structure. This is a status message only.
This isolated bond is probably not intended to have chemical significance.	Displayed for unlabeled single bonds unattached to other bonds. All bonds are interpreted chemically, usually as C_2H_6, and may cause unexpected results if intended as a graphical line only. This is a status message only.
The atom is very close to another atom or bond.	Displayed for any atom that is nearly touching another atom or bond but not bound to it. If a bond really was intended, the analysis of the structure produces incorrect results. This is s status message only.
The stereocenter has no stereobonds specified.	Displayed for any asymmetric center without attached wedged, hashed, dashed, or bold bonds. This is a status message only, and appears only when Show Stereochemistry is tuned on and there is at least one other wedged, hashed, dashed, or bold bond in the structure.
There is a valence and charge error somewhere in this aromatic system.	Displayed for any odd-membered ring drawn as a delocalized system (with a circle in the middle), where there is no corresponding associated charge. For example, a delocalized representation of cyclopentadiene must include either a negative charge or a multicenter attachment.
The stereocenter has conflicting or ambiguous stereobonds specified.	Displayed for any stereocenter (tetrahedral atom, asymmetric double bond, etc.) where the absolute stereochemistry cannot be determined from the structure as drawn. For example, this message would be shown for a carbon atom attached by bold bonds to four different ligands. This message is displayed only when Show Stereochemistry is also turned on.

Message	Description
This label has an unrecognized isotopic mass.	Displayed for every label that has a numeric superscript immediately preceding an atomic symbol, where the superscripted number does not correspond to a recognized isotope. For example, $^{24}CH_3$.

Appendix D: Ultra How ChemNMR Works

Overview

ChemNMR estimates chemical shifts for all hydrogen or carbon atoms for which additivity rules are available. Following a hierarchical list, it first identifies key substructures of a molecule. A substructure provides the base value for the estimated shift. For example, benzene would be identified as the key substructure of trinitrotoluene.

When a substructure happens to be a ring system not available in the data, ChemNMR approximates its base shift using embedded rings and, if necessary, it will even disassemble the ring into acyclic substructures.

ChemNMR views remaining parts of the molecule as substituents of a substructure. Each substituent adds to or subtracts from the base shift of the substructure to which it is attached. Additivity rules determine the increment of each contribution. If an increment for a substituent cannot be determined, ChemNMR uses embedded substituents—smaller structural units with the same neighboring atoms. Or, it will use increments of identical or embedded substituents of a corresponding substructure by assuming that the effects of the substituents are of the same magnitude.

ChemNMR provides a detailed protocol of the estimation process applied. It gives substructures as names, compound classes in most cases, substituents in form of a linear code, respectively.

The data set for the ^{1}H NMR Shift tool currently contains 700 base values and about 2000 increments. The ^{13}C NMR Shift tool is based on 4000 parameters. It also implements models for ethylenes (cis/trans) and cyclohexanes (equatorial/axial).

ChemNMR Limitations

The program handles the following elements:

H, D, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, Ac, Th, Pa, U, Nep, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr. Functional groups are expanded automatically.

In case of ^{1}H NMR, it estimates shifts of about 90% of all CH_x-groups with a standard deviation of 0.2. 0.3 ppm. The use of polar solvents may strongly increase these deviations. It does not estimate shifts of hydrogen atoms bonded to heteroatoms because they are significantly affected by solvents, concentration, impurities, and steric effects.

In case of ^{13}C NMR, it estimates over 95% of the shifts with a mean deviation of -0.29 ppm and standard deviation of 2.8 ppm.

For more information see:

Fürst, A.; Pretsch, E. *Anal. Chim. Acta* **1990**, *229*, 17.

Pretsch, E.; Fürst, A.; Badertscher M.; Bürgin, R.; Munk, M. E. *J. Chem. Inf. Comp. Sci.* **1992**, *32*, 291-295.

Bürgin Schaller, R.; Pretsch, E. *Anal. Chim. Acta* **1994**, *290*, 295.

Bürgin Schaller, R.; Arnold, C.; Pretsch, E. *Anal. Chim. Acta* **1995**, *312*, 95-105.

Bürgin Schaller, R.; Munk, M. E.; Pretsch, E. *J. Chem. Inf. Comput. Sci.***1996**, *36*, 239-243.

Appendix E: Pro How ChemProp Works

ChemProp Values

ChemProp enables you to calculate predicted values of selected physical and thermodynamic properties for structures of up to 100 atoms. The following topics describe how ChemProp obtains its values.

LogP

LogP (partition coefficient for *n*-octanol/water)—three fragmentation methods are used to predict the logP values.

Method one is based on 94 atomic contributions evaluated from 830 molecules by least squares analysis. This method works with a standard deviation of 0.47 logP units and can handle molecules containing hydrogen, oxygen, nitrogen, sulfur and halogens.

1. Method two is an extension of method one that is based on 120 atomic contributions evaluated from 893 molecules by least squares analysis. In addition to the atoms introduced for method one, it can handle molecules that contain phosphorus and selenium atoms. This method works with a standard deviation of 0.50 logP units.
2. Method three is based on 222 atomic contributions calculated from 1868 molecules by least squares analysis. This method allows a calculation of logP with a standard deviation of 0.43 logP units and can handle molecules containing hydrogen, oxygen, nitrogen, sulfur, halogens and phosphorus atoms. If this method is applied to molecules with internal hydrogen bonds, the standard deviation is 0.83 logP units.

Henry's Law

Henry's Law Constant—The air to water partition coefficient that is expressed as ratio of vapor pressure to water solubility or as a unitless distribution coefficient that can be evaluated as a ratio of the concentration in air to the concentration in water.

Two methods are used to predict Henry's Law constant.

1. The first is an approach based on the bond contribution method. This method uses 59 bond contribution values and 15 correction factors. The contributions were calculated by least squares analysis using a data set of 345 chemicals. This method estimates with a mean error of 0.30 units and a standard deviation of 0.45 units and can handle molecules containing carbon, hydrogen, oxygen, nitrogen, sulfur, phosphorus and halogens.
2. In the second method, Henry's Law constant is estimated from an equation found using linear regression. Multifunctional compounds were omitted from this study. This method should not be used for compounds where distant polar interaction is present.

Molar Refractivity

Molar refractivity—Two fragmentation methods are used to estimate the molar refractivity value.

1. Method one includes 93 atomic contributions evaluated from 504 molecules by using a constrained least squares technique. This method works with a standard deviation 1.27 cm^3/mol and can handle molecules containing hydrogen, oxygen, nitrogen, sulfur and halogens.
2. The second method is an extension of method one that includes 120 atomic contributions evaluated from 538 molecules by using a constrained least squares analysis technique. In addition to the atoms introduced for method one, this method can handle molecules with phosphorus and selenium atoms. This method works with a standard deviation of 0.77 cm^3/mol.

Ultra ClogP and CMR

Specific algorithms for calculating LogP and molar refractivity from fragment-based methods developed by the Medicinal Chemistry Project and BioByte.

For more information, see: biobyte.com

Topological Polar Surface Area

The polar surface area of a molecule (measured in square Ångstroms) is an imporant property that can be used for the prediction of pharmaceutical transport properties in the body. Historically, this property has been calculated using time-consuming 3D techniques, but a recent paper[1] has provided a remarkably accurate way of predicting it very rapidly. ChemDraw implements this algorithm, and displays it on the Chemical Properties window.

Other Properties

Heat of Formation, **Gibbs Free Energy**, **Ideal Gas Thermal Capacity**, **Freezing Point**, **Critical Temperature**, **Critical Pressure**, and **Critical Volume** are estimated using Joback's fragmentation method.

Normal Boiling Point and Melting Point— Estimated in K using two methods.

1. Joback's fragmentation method.
2. The Joback method as modified by Stein. All boiling points are estimated at a pressure of 1 atm.

1. Ertl, P., Rohde, B., and Selzer, P., 2000. Fast Calculation of Molecular Polar Surface Area as a Sum of Fragment Based Contributions and Its Application to the Prediction of Drug Transport Properties. *J.Med. Chem.*43: 3714-3717.

Appendix F: Shortcuts and Hotkeys

Shortcuts are key sequences used by power users to save time. The following tables list the ChemDraw shortcuts.

ChemDraw Hotkeys are used for rapid labeling of atoms, and for applying atom and bond properties. The tables list the default ChemDraw Hotkeys. See "Labeling Atoms with HotKeys" on page 87 for information on customizing Hotkeys.

ChemDraw Windows Shortcuts

See also "ChemDraw Hotkeys" on page 252.

File Commands

Enter...	to execute Command...
Ctrl+N	new document
Ctrl+O	open document
Ctrl+W	close document
Alt+F4	exit
Ctrl+S	save document
Shift+Ctrl+S	save as…
Shift+Ctrl+P	page set up…
Ctrl+P	print…

Edit Commands

Enter...	to execute Command...
Ctrl+Z	undo
Ctrl+X	cut
Ctrl+C	copy
Ctrl+V	paste
Shift+Ctrl+Z	redo
Del	clear
Ctrl+A	select all
Ctrl+Y	repeat last command

View Commands

Enter...	to execute Command...
F5	actual size
F6	fit to window
F7	magnify
F8	reduce
F11	toggle rulers
Ctrl+H	toggle crosshair

Object Commands

Enter...	to execute Command...
F2	bring to front
F3	send to back
Ctrl+E	toggle fixed angles
Ctrl+G	group selected objects
Shift+Ctrl+G	ungroup objects
Shift+Ctrl+H	flip horizontal
Alt+Shift+H	rotate 180° horizontal
Ctrl+J	join selected objects
Ctrl+K	scale selected object
Ctrl+L	toggle fixed lengths
Ctrl+R	rotate
Shift+Ctrl+V	flip vertical
Alt+Shift+V	rotate 180° vertical
Shift+Click (*with Lasso, Marquee, or Structure Perspective tools*)	select multiple objects

Structure Commands

Enter...	to execute Command...
Shift+Ctrl+K	clean up structure
Shift+Ctrl+N	convert name to structure
Alt+Shift+Ctrl+N	convert structure to name

Text Commands

Enter...	to execute Command...
F9 (*in a label*)	subscript the selected character or the next character typed

Enter...	to execute Command...
F10 (*in a label*)	superscript the selected character or the next character typed
Shift+Ctrl+C	centered
Shift+Ctrl+J	justified
Shift+Ctrl+L	flush left
Shift+Ctrl+M	automatic justification
Shift+Ctrl+R	flush right

Help Commands

Enter...	to execute Command...
F1	Help contents
Shift+F1	context sensitive Help

Drawing Commands

Enter...	to execute Command...
Shift+click (*with saturated double bond ring tools*)	change orientation of double bonds
Ctrl+click (*with ring tools except chairs*)	create resonance delocalized ring
Alt+Shift+click (*with pen tool*)	remove a curve segment
Shift+drag (*with resize handle*)	distort (limit resize to X or Y axis
Ctrl+drag	copy a selected object
Ctrl+drag (*with alkane chain tool*)	change direction of a chain
Shift+Ctrl+drag	copy a selected object (constrained to X and Y axes)
Ctrl+Alt+Tab	toggles the Lasso and the previous drawing tool

ChemDraw Mac Shortcuts

See also "ChemDraw Hotkeys" on page 252.

File Commands

Enter...	to execute Command...
Command+M	minimize the ChemDraw window
Command+N	new document

Enter...	to execute Command...
Command+O	open document
Command+P	print…
Shift+Command+P	page set up…
Command+Q	quit
Command+S	save document
Shift+Command+S	save as…
Command+W	close document

Edit Commands

Enter...	to execute Command...
Command+A	select all
Command+C	copy
Command+V	paste
Command+X	cut
Command+Y	repeat last command
Command+Z	undo
Del	clear

View Commands

Enter...	to execute Command...
Command+H	toggle crosshair
Command+\	actual size
Command+/	fit to window
Command+>	magnify
Command+<	reduce
Command+;	toggle rulers

Object Commands

Enter...	to execute Command...
Command+E	toggle fixed angles
Command+G	group selected objects
Shift+Command+G	ungroup objects
Shift+Command+H	flip horizontal
Option+Shift+ Command+H	rotate 180° horizontal
Command+J	join selected objects
Command+K	scale

Enter...	to execute Command...
Command+L	toggle fixed lengths
Command+R	rotate
Shift+Command+V	flip vertical
Option+Shift+ Command+V	rotate 180° vertical
Command+[	bring to front
Command+]	send to back
Shift+Click	select multiple objects

Structure Commands

Enter...	to execute Command...
Shift+Command+K	clean up structure
Shift+Command+N	convert name to structure
Option+Command+N	convert structure to name

Text Commands

Enter...	to execute Command...
Shift+Command+C	centered
Shift+Command+J	justified
Shift+Command+L	flush left
Shift+Command+M	automatic justification
Shift+Command+R	flush left
Shift+Option+8 (*in a label*)	insert ° symbol

Drawing Commands

Enter...	to execute Command...
Shift+click (*with saturated double bond ring tools*)	change orientation of double bonds
Command+click (*with ring tools except chairs*)	create resonance delocalized ring
Option+Shift+click (*with the pen tool*)	remove a curve segment
Shift+drag (*with resize handle*)	distort (limit resize to X or Y axis)
Command+drag	copy a selected object
Command+drag (*with alkane chain tool*)	change direction of a chain
Shift+Command+drag	copy a selected object (constrained to X and Y axes)

Enter...	to execute Command...
Command+Option+Tab	toggles the Lasso and the previous drawing tool

ChemDraw Hotkeys

Hotkeys are used for rapid labeling of atoms, and for applying atom and bond properties. The following tables list the default ChemDraw Hotkeys. See "Labeling Atoms with HotKeys" on page 87 for information on customizing Hotkeys.

See also"ChemDraw Windows Shortcuts" on page 247

Atom Hotkeys

NOTE: *All Hotkeys can be edited except <Enter> or <Return>, <Space>, <Backspace>, and <Delete>.*

Hotkey	Result
a	A
A or 5	Ac
b	Br
c	C
C or l (*lower case L*)	Cl
d	D
e	Et
E	$COOCH_3$
f	F
h	H
i	I
k	K
l	Cl
m	Me
n	N
N	Na
o	O
p	P
P or 4	Ph
q	Q (*non-hydrogen heteroatom*)
r	R
s	S
S	Si
t	TMS

Hotkey	Result
T	OTs
x	X
1	n-Bu
2	s-Bu
3	t-Bu
4	Ph
5	Ac
<Enter>	Open an atom label text box.
/ (*slash*)	Display the **Atom Properties** dialog box.
= (*equals*)	Display the **Choose Nickname** dialog box.
. (*period*)	Add an attachment point.
‘ (*single quote*)	Add an atom number.
<space>	Remove an atom label.
<Backspace> or <Delete>	Remove an atom label or bond.

Bond Editing Hotkeys

Hotkey	Result
1	Change to single bond.
2	Change to double bond.
3	Change to triple bond.
4	Change to quadruple bond.
c	Center a double bond.
l	Position a double bond to the left.
r	Position a double bond to the right.
f	Bring a bond to the front.

Appendix G: Document Settings

Creating Style Sheets or Stationery Pads

To create your own Style Sheet or Stationery Pad:

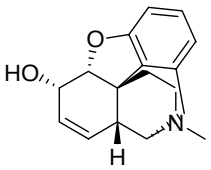
1. Create a new document.
2. Enter the settings in the **Page Setup**, **Drawing**, **Text Settings**, and **Color Palette** dialog boxes.
3. From the File menu, choose **Save As**.
4. In the Save As dialog box:
   a. Select the CD Style Sheet or Stationery Pad file format.
   b. Type a name for the document.
   c. Select the **ChemDraw Items** folder as the location for saving the template.
5. Click **OK** or **Save**.

ChemDraw Style Sheets or Stationery Pads

This following table contains drawing settings and a sample structure for each of the Style Sheets or Stationery Pads ChemDraw provides.

Drawing, Atom Label, and Caption Text Settings in Journal Style Sheets or Stationery Pads

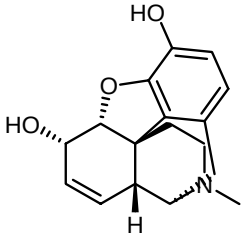
ACS 1996



Morphine

- Fixed Length: **14.4 pt**
- Bold Width: **2 pt**
- Line Width: **0.6 pt**
- Margin Width: **1.6 pt**
- Hash Spacing: **2.5 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **18**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **10 pt**
- Drawing Area (Width x Height): **540 pt x 720 pt**
- Page Size: **US Letter**
- Reduction (%): **100**

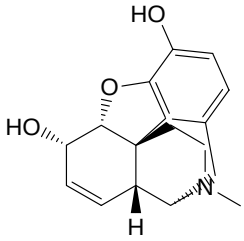
Adv. Synth. Catal.



Morphine

- Fixed Length: **17 pt**
- Bold Width: **2 pt**
- Line Width: **1 pt**
- Margin Width: **1.6 pt**
- Hash Spacing: **2.5 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **18**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Times New Roman/Times**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **540 pt x 720 pt**
- Page Size: **US Letter**
- Reduction (%): **100**

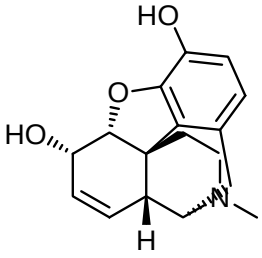
Helvetica Chimica Acta



Morphine

- Fixed Length: **17 pt**
- Bold Width: **2.9 pt**
- Line Width: **0.54 pt**
- Margin Width: **2 pt**
- Hash Spacing: **2 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length):**14**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **368 x 720 pts**
- Page Size: **US Letter**
- Reduction (%): **100**

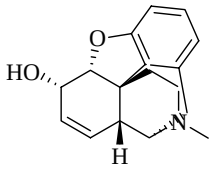
J. Chin. Chem. Soc.



Morphine

- Fixed Length: **18 pt**
- Bold Width: **2.5 pt**
- Line Width: **1 pt**
- Margin Width: **2 pt**
- Hash Spacing: **2.5 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **20**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **12 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **693 pt x 918 pt**
- Page Size: **US Letter**
- Reduction (%): **80**

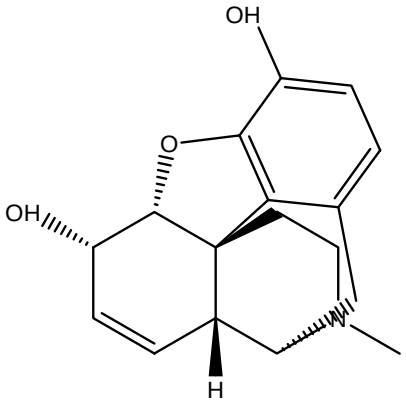
J. Mol. Med.



Morphine

- Fixed Length: **14.4 pt**
- Bold Width: **2 pt**
- Line Width: **0.6 pt**
- Margin Width: **1.6 pt**
- Hash Spacing: **2.5 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **18**
- Atom Label Font (Win/Mac): **Times New Roman/Times**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): Times New Roman/Times
- Caption Size: **10 pt**
- Drawing Area (Width x Height): **8.5 cm x 25.4 cm** (1 column)**; 17 cm x 25.4 cm** (2 column)
- Page Size: **US Letter**
- Reduction (%): **100**

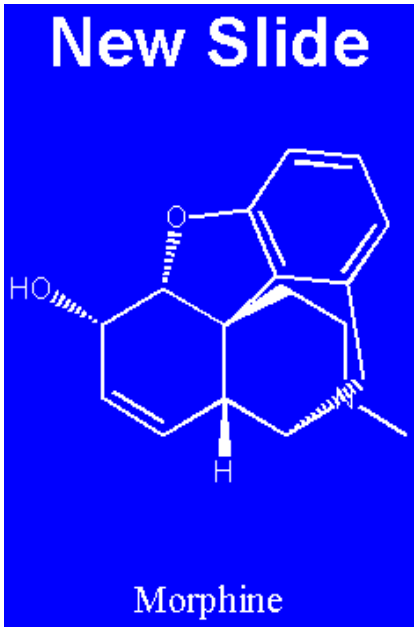
New Document



Morphine

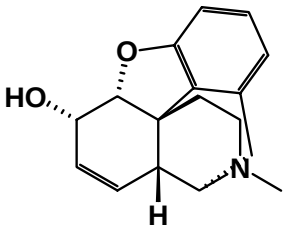
- Fixed Length: **30 pt**
- Bold Width: **2 pt**
- Line Width: **1 pt**
- Margin Width: **2 pt**
- Hash Spacing: **2.7 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **12**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Times New Roman/Times**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **7.5 in x 10 in**
- Page Size: **US Letter**
- Reduction (%): **100**

Drawing, Atom Label, and Caption Text Settings in Journal Style Sheets or Stationery Pads



- Fixed Length: **30 pt**
- Bold Width: **4 pt**
- Line Width: **1.6 pt**
- Margin Width: **2 pt**
- Hash Spacing: **2.7 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **15**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **12 pt**
- Caption Font (Win/Mac): **Times New Roman/Times**
- Caption Size: **16 pt**
- Drawing Area (Width x Height): **7.5 in x 10 in**
- Page Size: **US Letter**
- Reduction (%): **100**

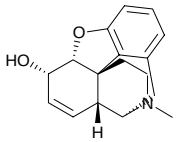
Phytomedicine



Morphine

- Fixed Length: **20 pt**
- Bold Width: **1.33 pt**
- Line Width: **1pt**
- Margin Width: **1.25 pt**
- Hash Spacing: **3 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **8**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **12 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **540 pt x 720 pt**
- Page Size: **US Letter**
- Reduction (%): **100**

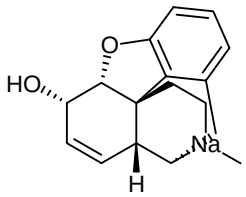
RSC (1 and 2 column)



Morphine

- Fixed Length: **0.43 cm**
- Bold Width: **0.056 cm**
- Line Width: **0.016 cm**
- Margin Width: **0.044 cm**
- Hash Spacing: **0.062 cm**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **20**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **9 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **9 pt**
- Drawing Area (Width x Height): **8.9 cm x 25.4 cm** (1 column); **19 cm x 27.7 cm**
- Page Size: **US Letter**
- Reduction (%): **100**

SYNTHESIS, SYNLETT



Morphine

- Fixed Length: **17 pt**
- Bold Width: **2 pt**
- Line Width: **0.8 pt**
- Margin Width: **1.3 pt**
- Hash Spacing: **2.5 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **18**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **10 pt**
- Drawing Area (Width x Height): **12 cm x 26.7 cm**
- Page Size: **A4**
- Reduction (%): **100**

Appendix H: Chemistry File Formats

Overview

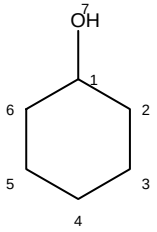
File formats other than ChemDraw may not preserve all of your data. ChemDraw can create many types of items—particularly graphical objects such as boxes and curves—that cannot be saved into chemical file formats.

Other file formats sometimes contain data that cannot be interpreted by ChemDraw. ChemDraw always tries to interpret other file formats so that as much chemically-relevant data is preserved as possible, even if that causes the actual appearance of the file to change when it is saved and reopened.

Most file formats supported by ChemDraw are proprietary or extremely complex and are documented more thoroughly elsewhere. For example, you can find more information about CambridgeSoft's CDX file format at: sdk.cambridgesoft.com

Connection Table File Format

The connection table format file described in this section is generated for the cyclohexanol structure shown below. All references to atom serial numbers are based on the Atom Numbering shown.



The following is a sample Connection Table file produced for cyclohexanol using ChemDraw. The line numbers are added for purposes of discussion only.

Line 1	Cyclohexanol			
Line 2	7 7			
Line 3	0.0000	0.5000	0.0000	C
Line 4	-0.8667	0.0000	0.0000	C
Line 5	-0.8667	-1.0000	0.0000	C
Line 6	0.0000	-1.5000	0.0000	C
Line 7	0.8667	-1.0000	0.0000	C
Line 8	0.8667	0.0000	0.0000	C
Line 9	0.0000	1.5000	0.0000	O
Line 10	1 2 1 1			
Line 11	2 3 1 1			
Line 12	3 4 1 1			
Line 13	4 5 1 1			
Line 14	5 6 1 1			
Line 15	1 6 1 1			
Line 16	6 7 1 1			

Each line represents a data record containing one or more fields of information about the structure. Individual fields are delimited by space(s) or a tab. The fields in the Connection Table format file used by ChemDraw are discussed below. The field value for Carbon 6 from the example file is included in parentheses for reference.

- Line 1 is the molecule name. The molecule name is the file name when the file was created using ChemDraw.

- Line 2 contains two fields: the first field is the number of atom labels, and the second field is the number of bonds. These fields must be separated by at least one space.
- Lines 3. 9 each contain 4 fields describing information about the individual atoms: the first field is the X Cartesian coordinate (0.8667), the second field is the Y Cartesian coordinate (0.0000), the third field is the Z Cartesian coordinate (0.0000), and the fourth field is the atom label (C).

  The spacing of these fields is very important. Any data outside the following columns (especially data overlapping the ranges) may render a file unreadable.
  - Field 1: Columns 0. 9
  - Field 2: Columns 10. 19
  - Field 3: Columns 20. 29
  - Field 4: Columns 31. end
- Lines 10. 16 each contain four fields describing information about the individual bonds between the atoms: the first two fields represent the serial numbers of the atoms that are connected by this bond (atom 1 and atom 6), the third field is the bond order (1) and the fourth field is the bond type (1).

The bond types for the Connection Table format are as follows:

value	bond type
1	Single.
2	Dashed.
3	Hashed.
4	Wedged hash with first atom at narrow end.
5	Wedged hash with second atom at narrow end.
6	Bold.
7	Wedged with first atom at narrow end.
8	Wedged with second atom at narrow end.
9	Wavy.
10	Hollow wedge with narrow end towards 1st atom.
11	Hollow wedge with narrow end towards 2nd atom.
12	Dative bond with arrow towards 2nd atom.
13	Dative bond with arrow towards 1st atom.
14	Any (bond property).
15	Single/Double (bond property).
16	Double/Aromatic (bond property).
17	Single/Aromatic (bond property).

Double bonds are bit encoded using a bitmask. The default value (0) indicates a normal (two solid lines) double bond, with the second line on the right (looking from the first atom to the second). Other values are as follows:

value	bond type/position
1	The second line is on the left (looking from the first atom to the second).
2	The two lines are centered.
4	A double bond with one dashed and one solid line.
8	A modifier to the previous two values, indicating that the user specifically set the positioning. If this bit is not present, ChemDraw calculated the positioning automatically.
16	A double bond with one bold and one solid line.
32	A crossed bond.
64	A double bond with two dashed lines.

So, for example, a bitmask value of 13 (= 1 + 4 + 8) means a double bond with one dashed and one solid line (4), where the user specifically wants (8) the second line to be on the left (1).

NOTE: *This connection table format is obsolete, and is documented here for historical purposes only. This format should never be used for critical work where chemical information is important.*

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Life Science Enterprise Solutions
Lösungen für biowissenschaftliche Unternehmen
Solutions d'entreprise Life Science
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Desktop Software
Enterprise Solutions
Research & Discovery
Applied BioInformatics
Knowledge Management
Chemical Databases
ChemDraw
ChemOffice

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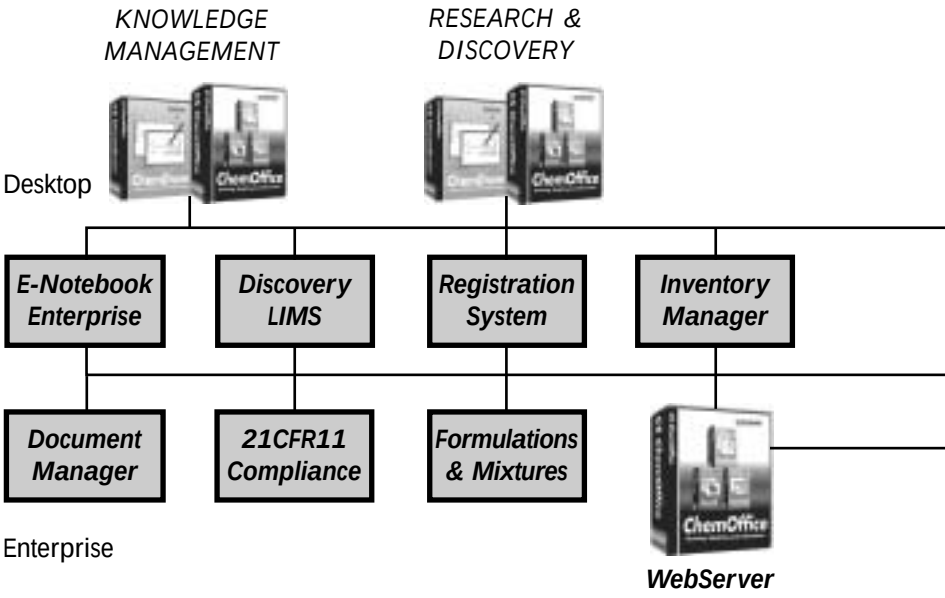
ChemOffice Desktop to



DESKTOP SOFTWARE

ChemOffice
E-Notebook
ChemDraw
Chem3D
ChemFinder
ChemInfo

Success begins at the desktop, where scientists use *ChemDraw* and *ChemOffice* to pursue their ideas and communicate with colleagues using the natural language of chemical structures, models, and information. In the lab, scientists capture their results by organizing chemical information, documents, and data with *E-Notebook*. *Chem3D* modeling and *ChemFinder* information retrieval integrate smoothly with *ChemOffice* and Microsoft Office to speed day-to-day research tasks.

ENTERPRISE SOLUTIONS

ChemOffice WebServer
Oracle Cartridge

Just as *ChemOffice* supports the daily work of the individual scientist, enterprise solutions and databases, built on *ChemOffice WebServer,* and *Oracle Cartridge* help organizations collaborate and share information.

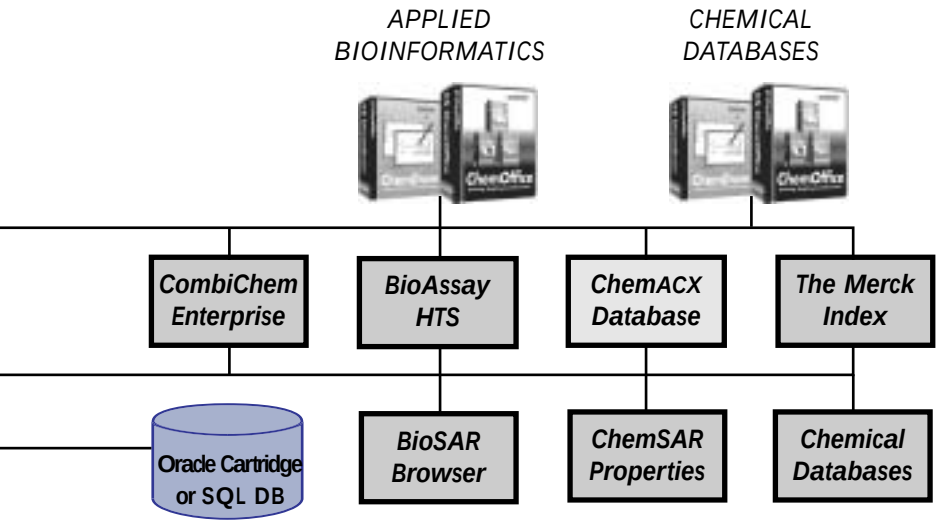
KNOWLEDGE MANAGEMENT

E-Notebook Enterprise
Document Manager
Discovery LIMS
21CFR11 Compliance

Research organizations thrive when information is easily captured, well organized, and available to others who need it. *E-Notebook Enterprise* streamlines daily record keeping with rigorous security and efficient archiving, and facilitates searches by text and structure. *Document Manager* organizes procedures and reports for archiving and chemically-intelligent data mining. *Discovery LIMS* tracks laboratory requests, and *21CFR11 Compliance* implements an organization's regulatory compliance processes.

SOLUTIONS

Enterprise Solutions



RESEARCH & DISCOVERY

Registration System
Formulations & Mixtures
Inventory Manager
CombiChem Enterprise

Managing the huge data streams of new lab technology is a key challenge. *Registration System* organizes information about new compounds according to an organization's business rules, while *Inventory Manager* works with *Registration System* and chemical databases for complete management of chemical inventories. *CombiChem Enterprise* and *Formulations & Mixtures* are also important parts of research data management.

APPLIED BIOINFORMATICS

BioAssay HTS
BioSAR Browser

Finding structural determinants of biological activity requires processing masses of biological assay data. Scientists use *BioAssay HTS* and *BioSAR Browser* to set up biological models and visualize information, to generate spreadsheets correlating structure and activity, and to search by structure.

CHEMICAL DATABASES

ChemACX Database
ChemSAR Properties
The Merck Index
Chemical Databases

Good research depends on reference information, starting with the structure-searchable *ChemACX Database* of commercially available chemicals. *The Merck Index* 13th Edition and other databases provide necessary background about chemicals, their properties, and reactions.

CONSULTING & SERVICES

Consulting Development
Support & Training

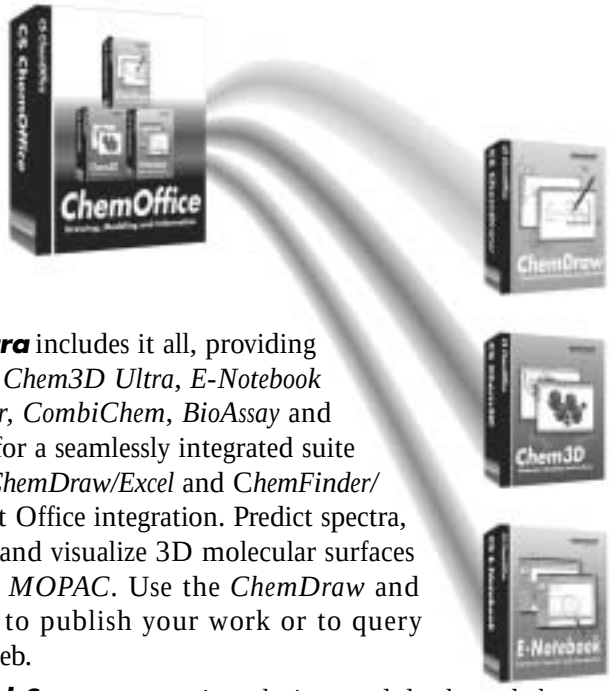
CambridgeSoft's scientific staff has the industry experience, and chemical and biological knowledge to maximize the effectiveness of your information systems.

CS ChemOffice

	Software Suites	ChemOffice Ultra	ChemOffice Pro	ChemDraw Ultra	ChemDraw Pro	ChemDraw Std	Chem3D Ultra	E-Notebook Ultra
	Includes							
Software	*ChemDraw Ultra	Win/Mac	■	■	■				
	*ChemDraw Pro	Win/Mac				■			
	*ChemDraw Std	Win/Mac					■	■	■
	*ChemDraw Plugin Pro	Win/Mac	■	■	■	■			
	*Chem3D Ultra	Win	■					■	
	*Chem3D Pro	Win		■					
	Chem3D Std	Win			■				■
	*Chem3D Plugin Pro	Win	■	■	■			■	
	*E-Notebook Ultra	Win	■						■
	ChemFinder Pro	Win	■	■					■
	ChemFinder Std	Win			■			■	
Applications & Features	ChemDraw/Spotfire	Win	■						
	*BioAssay Pro	Win	■						
	Purchase/Excel	Win	■						
	CombiChem/Excel	Win	■	■	■				■
	ChemFinder/Office	Win	■	■	■				■
	ChemDraw/Excel	Win	■	■	■				■
	Name=Struct	Win/Mac	■	■	■				
	Struct=Name	Win/Mac	■	■	■				
	ChemNMR	Win/Mac	■	■	■				
	CLogP/ChemDraw	Win/Mac	■	■	■				
	BioArt	Win/Mac	■	■	■				
	Structure Clean Up	Win/Mac	■	■	■	■			
	Polymer Draw	Win/Mac	■	■	■	■			
	LabArt	Win/Mac	■	■	■	■	■	■	■
	ChemSAR/Excel	Win	■	■				■	
	3D Query	Win	■	■					
	MOPAC/Chem3D	Win	■					■	
	GAMESS Client	Win	■					■	
	Gaussian Client	Win	■					■	
	Tinker/Chem3D	Win	■					■	
	*CAMEO/ChemDraw	Win							
Databases	*The Merck Index	Win	■						
	*ChemACX Ultra	Win	■						
	ChemSCX	Win	■						
	ChemMSDX	Win	■						
	*ChemINDEX Ultra	Win	■	■					■
	ChemRXN	Win	■	■					■
	NCI & AIDS	Win	■	■					■

*Available Separately

Desktop to Enterprise Solutions



ChemOffice Ultra includes it all, providing *ChemDraw Ultra, Chem3D Ultra, E-Notebook Ultra, ChemFinder, CombiChem, BioAssay* and *The Merck Index*, for a seamlessly integrated suite for chemists.Use *ChemDraw/Excel* and *ChemFinder/Word* for Microsoft Office integration. Predict spectra, use *Name=Struct*, and visualize 3D molecular surfaces and orbitals with *MOPAC*. Use the *ChemDraw* and *Chem3D Plugins* to publish your work or to query databases on the web.

ChemOffice WebServer enterprise solutions and databases help organizations collaborate on shared information with *ChemDraw* web-based interface and *Oracle Cartridge* security.

Knowledge Management with *E-Notebook Enterprise* streamlines daily record-keeping with rigorous security and efficient archiving. *Document Manager* indexes chemical structure content of documents and folders.

Research & Discovery efforts are improved with *Registration System* by organizing new compound information, while *Inventory Manager* works with chemical databases for complete management of chemical inventories.

Applied BioInformatics scientists use *BioAssay HTS* and *BioSAR Browser* to set up biological models and visualize information, to generate spreadsheets correlating structure and activity, and to search by structure.

Chemical Databases include the *ChemACX Database* of commercially available chemicals, *The Merck Index* 13th edition, and other databases.

Consulting & Services includes consulting development, technical support, and education training for pharmaceutical, biotechnology, and chemical customers, including government and education, by CambridgeSoft's experienced staff.

ChemOffice WebServer

Enterprise Solutions & Databases

- *Oracle Cartridge & Database Webserver*

Knowledge Management

- *E-Notebook Enterprise*, *Document Mgr*, *Discovery LIMS & 21CFR11 Compliance*

Research & Discovery

- *Registration System*, *Formulations & Mixtures*, *Inventory Manager & CombiChem Enterprise*

Applied BioInformatics

- *BioAssay HTS & BioSAR Browser*

Chemical Databases

- *The Merck Index*, *ChemACX & ChemSAR Properties*

ChemOffice Ultra

Ultimate Drawing, Modeling & Information

- Adds *The Merck Index, E-Notebook*, *CombiChem*, *MOPAC*, *BioAssay & ChemACX* to *Office Pro*

ChemOffice Pro

Premier Drawing, Modeling & Information

- Includes *ChemDraw Ultra*, *Chem3D Pro*, *ChemSAR/Excel*, *ChemFinder Pro*, *ChemINDEX & ChemRXN* databases

Also Available Separately...

ChemDraw Ultra

Ultimate Drawing, Query & Analysis

- Adds *ChemDraw/Excel, ChemNMR, Name=Struct, AutoNom & ChemFinder / Word* to *ChemDraw Pro*
- *ChemNMR*, Stereochemistry, Polymers & *BioArt*

ChemDraw Pro

Premier Drawing & Database Query

- Define complex database queries
- ISIS/Draw & Base compatible via copy/paste
- *Structure CleanUp* and Chemical Intelligence

Chem3D Ultra

Ultimate Modeling, Visualization & Analysis

- Adds *MOPAC*, *CLogP*, *Tinker, ChemProp*, *ChemSAR & Chem3D Plugin* to *Chem3D Pro*
- Advanced modeling & molecular analysis tool

E-Notebook Ultra

Ultimate Journaling & Information

- *E-Notebook, ChemDraw Std, Chem3D Std, ChemDraw/Excel & CombiChem/Excel*
- Includes *ChemFinder, ChemFinder/Word, ChemINDEX & ChemRXN* databases

Some features are Windows only.
All specifications subject to change without notice.

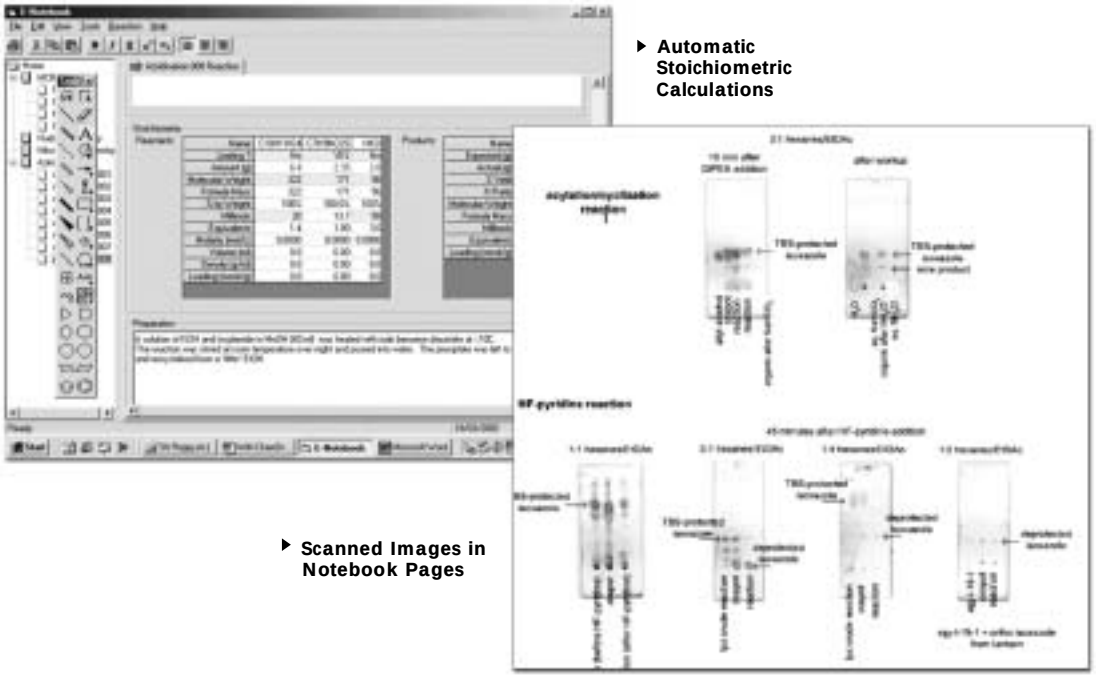
CS E-Notebook

Electronic Journal and Information

E-Notebook Ultra streamlines daily record keeping tasks of research scientists, maintains live chemical structures and data, and saves time documenting work and retrieving chemical information. *E-Notebook* combines all of your notebooks into one and sets up as many project notebooks as you need, organized the way you work. Notebook pages include *ChemDraw* documents, Excel spreadsheets, Word documents and spectral data. *E-Notebook* automatically performs stoichiometry calculations on *ChemDraw* reaction pages. Search by structure, keyword, dates and other types of data. Maintain required hardcopy archives by printing out pages. Information cannot be accidentally modified. Spectral controls from Thermo Galactic are available.

CombiChem/Excel builds combinatorial libraries with embedded *ChemDraw* structures using *ChemDraw/Excel* for Windows. Find reagents with *ChemFinder* and design experiments.

BioAssay Pro, available in *ChemOffice Ultra*, allows for flexible storage and retrieval of biological data. It is designed for complex lead optimization experiments and supports almost any biological model.

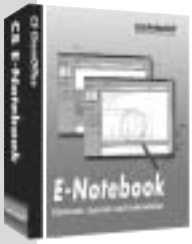


▸ **Automatic Stoichiometric Calculations**

▸ **Scanned Images in Notebook Pages**

E-Notebook Ultra

Ultimate Journaling & Information



- Advanced search and structure query features
- Stores structures and models for easy retrieval
- Stores physical and calculated data
- Search by substructure, including stereochemistry, using *ChemDraw*
- Search and store chemical reaction data
- *CombiChem/Excel* combinatorial libraries
- Integration with *ChemDraw* and *Chem3D*
- Import/export MDL SD & RD files

CombiChem/Excel

Combinatorial Chemistry in Excel

- Generate combinatorial libraries
- Choose starting materials & reaction schemes
- View structures & track plate/well assignments

ChemFinder Pro

Premier Searching & Information

- Advanced search & structure query features
- Stores structures & reactions along with calculated data & associated information
- Search by substructure including stereochemistry using *ChemDraw*
- Integration with *ChemDraw* & *Chem3D*
- Import/export MDL SD & RD files

ChemInfo Std

Reference & Reaction Searching

- *ChemINDEX* for small molecule information
- *ChemRXN* for reaction databases

BioAssay Pro

Biological Assay Structure Activity

- Set up biological models & visualize information
- Search data by structure to isolate key structural determinants of biological activity
- Tabulate & analyze structure-activity relationships with spreadsheet templates
- Available in *ChemOffice Ultra*

SYSTEMS & LANGUAGES

English & Japanese
Windows: 95, 98, Me, NT, 2000, XP
This software is Windows only.
All specifications subject to change without notice.

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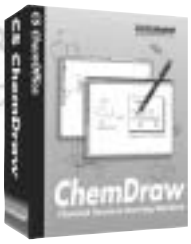
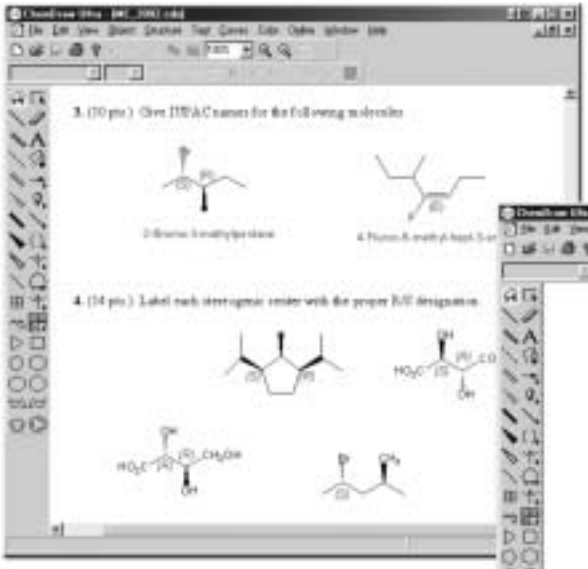
CS ChemDraw

Chemical Structure Drawing Standard

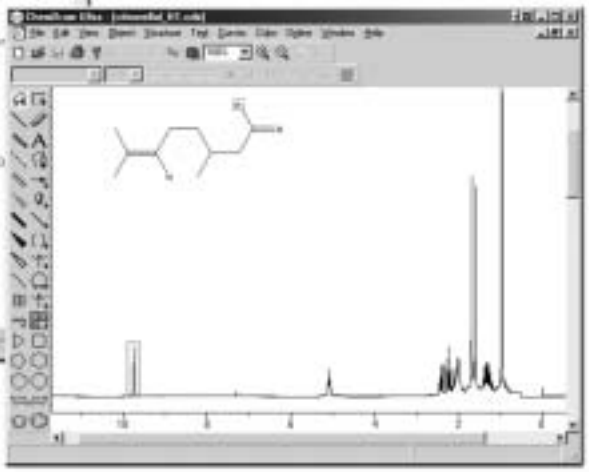


ChemDraw Ultra adds *ChemDraw/Excel*, *ChemNMR*, *Name=Struct*, Beilstein's *AutoNom*, *CLogP* and *ChemFinder/Word* to *ChemDraw Pro*. With rich polymer notation, atom numbering, *BioArt* templates, and modern user interface, *ChemDraw* is more powerful than ever before. Create tables of structures, identify and label stereochemistry, estimate NMR spectra from a *ChemDraw* structure with structure-to-spectrum correlation, obtain structures from chemical names, assign names from structures, and create multi-page documents and posters.

ChemDraw Pro will boost your productivity more than ever. Draw publication-quality structures and reactions. Publish on the web using the *ChemDraw Plugin*. Create precise database queries by specifying atom and bond properties and include stereochemistry. Display spectra, structures, and annotations on the same page. Use the *Online Menu* to query *ChemACX.Com* by structure, identify available vendors, and order online.



▸ **Stereochemistry**



▸ **Structure-to-Spectrum NMR Correlation**

ChemDraw Ultra

Ultimate Drawing, Query & Analysis

- Adds *ChemDraw/Excel, ChemNMR, Name=Struct, AutoNom & ChemFinder/Word* to *ChemDraw Pro*
- *Name=Struct/AutoNom* creates structures from names & vice versa
- *ChemNMR* predicts ^{1}H & ^{13}C NMR line spectra with peak-to-structure correlation
- Polymer notation based on IUPAC standards
- *ChemDraw/Excel* brings chemistry to Excel

ChemDraw Pro

Premier Drawing & Information Query

- Query databases precisely by specifying atom & bond properties, reaction centers, substituent counts, R-groups & substructure
- Read ISIS files with Macintosh/Windows cross-platform compatibility
- *Structure Clean Up* improves poor drawings
- Display spectra from SPC and JCAMP files
- Chemical intelligence includes valence, bonding & atom numbering
- Right-button menus speed access to features

ChemDraw Std

Publication Quality Structure Drawing

- Draw and print structures & reactions in color, and save as PostScript, EPS, GIF, SMILES & more
- Collections of pre-defined structure templates
- Large choice of bonds, arrows, brackets, orbitals, reaction symbols & *LabArt*
- Style templates for most chemical journals
- Compatible with *Chem3D*, *ChemFinder*, *ChemInfo, E-Notebook* & Microsoft Office

ChemDraw Plugin

Advanced WWW Structure Client

- Embed live *ChemDraw* documents in WWW pages
- Works with Netscape & Internet Explorer
- Included with *ChemDraw Ultra & Pro*

SYSTEMS & LANGUAGES

Windows & Macintosh English, Japanese, French, German
Windows: 95, 98, Me, NT, 2000, XP
Macintosh: MacOS 8.6-10.1
Some features are Windows only.
All specifications subject to change without notice.

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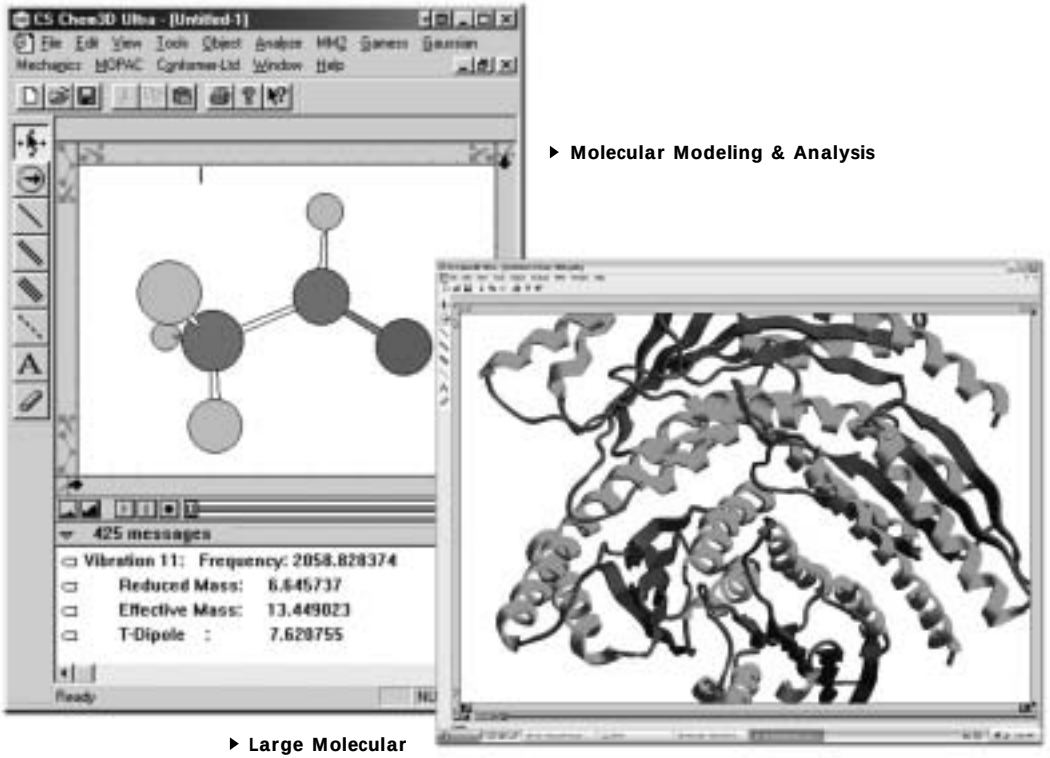
CS Chem3D

Molecular Modeling and Analysis

Chem3D Ultra includes *MOPAC*, *Tinker* and set-up/control interfaces for optional use of GAMESS and Gaussian. Estimate advanced physical properties with *CLogP* and *ChemProp*, and create SAR tables using property servers to generate data for lists of compounds. Use *ChemSAR/Excel* to explore structure activity relationships and use add-on *Conformer* for conformational searching. Publish and view models on the web using the *Chem3D Plugin*.

Chem3D Pro brings workstation quality molecular visualization and display to your desktop. Convert *ChemDraw* and ISIS/Draw sketches into 3D models. View molecular surfaces, orbitals, electrostatic potentials, charge densities and spin densities. Use built-in extended Hückel to compute partial atomic charges. Use MM2 to perform rapid energy minimizations and molecular dynamics simulations. *ChemProp* estimates physical properties such as logP, boiling point, melting point and more. Visualize Connolly surface areas and molecular volumes.



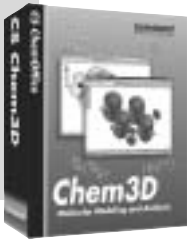
▸ **Molecular Modeling & Analysis**

▸ **Large Molecular Visualization**

Chem3D Ultra

Ultimate Modeling, Visualization & Analysis

- Adds *MOPAC*, *CLogP*, *Tinker, ChemProp*,*ChemSAR & Chem3D Plugin* to *Chem3D Pro*
- Includes GAMESS & Gaussian client interfaces
- *ChemSAR/Excel* builds SAR tables



Chem3D Pro

Premier Modeling, Visualization & Analysis

- Create 3D models from *ChemDraw* or ISIS Draw, accepts output from other modeling packages
- Model types: space filling CPK, ball & stick, stick, ribbons, VDW dot surfaces & wire frame
- Compute & visualize partial charges, 3D surface properties & orbital mapping
- Polypeptide builder with residue recognition
- *ChemProp*—Basic property predictions with Connolly volumes & surface areas
- MM2 minimization & molecular dynamics, extended Hückel MO calculations
- Supports: PDB, MDL Molfile, Beilstein ROSDAL, Tripos SYBYL MOL, EPS, PICT, GIF, 3DMF, TIFF, PNG & more

MOPAC/Chem3D

Advanced Semi-Empirical Computation

- Calculate ΔH_f, solvation energy, dipoles, charges, UHF & RHF spin densities, MEP, charge densities & more
- Optimize transition state geometries
- AM1, PM3, MNDO & MINDO/3 methods

CAMEO/ChemDraw

Synthetic Reaction Prediction

- Expert system predicts and displays products
- *ChemDraw* creates starting materials when you choose reaction conditions; sold separately

Chem3D Plugin

Advanced WWW Model Client

- Works with Microsoft Internet Explorer
- Visualize 3D molecules on *ChemFinder.Com*

SYSTEMS & LANGUAGES

Windows & Macintosh English & Japanese
Windows: 95, 98, Me, NT, 2000, XP
Macintosh: MacOS 8.6-9.2.X
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CS ChemFinder

Searching and Information Integration

ChemFinder Pro is a fast, chemically intelligent, relational database search engine for personal, group or enterprise use. Extended integration with Microsoft Excel and Word adds chemical searching and database capability to spreadsheets and documents.

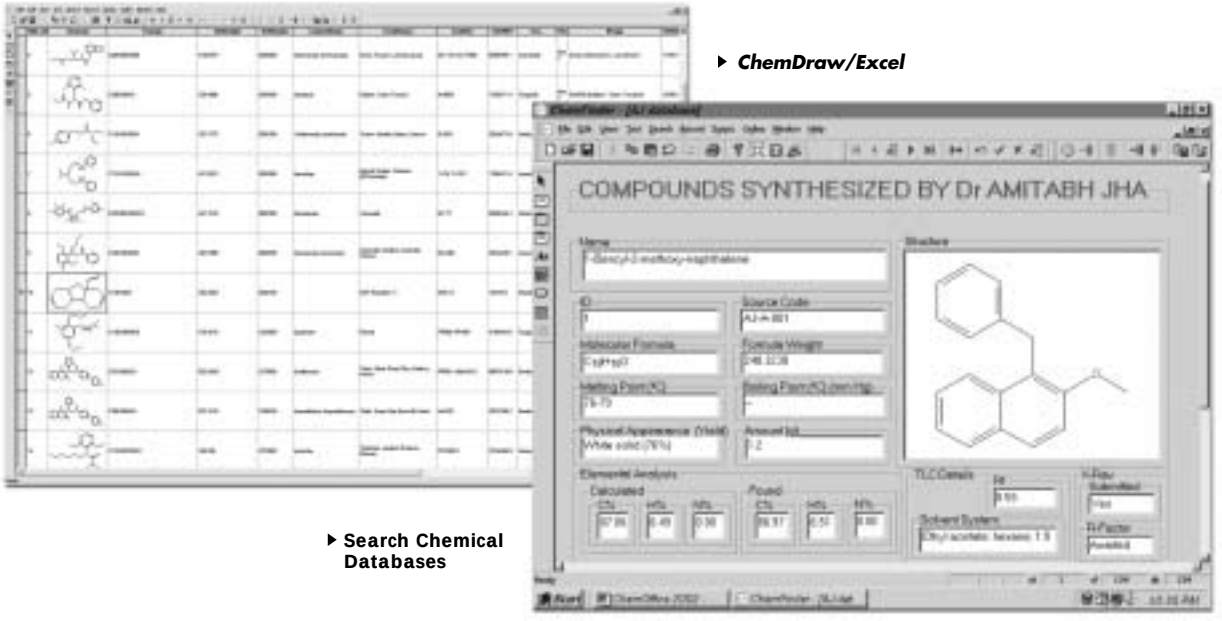
An ever-increasing number of chemical databases are available in *ChemFinder* format. Compatibility with MDL ISIS databases is provided by SDfile and RDfile import/export. *ChemFinder* provides network server workgroup functionality when used with *ChemOffice WebServer.*

ChemFinder/Word is an extension of Microsoft Excel and Word for Windows. Create structure searchable spreadsheets and index documents with embedded *ChemDraw* structures.

ChemDraw/Excel adds chemical intelligence to Microsoft Excel for Windows. Show structures in spreadsheet cells, tabulate chemical calculations and analyze data with Excel functions and graphs.

Purchase/Excel uses *ChemDraw/Excel* to manage reagent lists and track purchasing information.

CombiChem/Excel builds combinatorial libraries with embedded *ChemDraw* structures using *ChemDraw/Excel* for Windows. Find reagents with *ChemFinder* and design experiments.



▸ ***ChemDraw/Excel***

▸ **Search Chemical Databases**

ChemFinder/Word
• Search structures in documents & folders
ChemDraw/Excel
• Add chemical intelligence to spreadsheets
Purchase/Excel
• Organize chemical purchasing information

ChemFinder Pro
Premier Searching & Information
- Advanced search and structure query features
- Stores structures and reactions along with calculated data and associated information
- Search by substructure including stereochemistry using *ChemDraw*
- Import/export MDL SD and RD files
- Integration with *ChemDraw* and *Chem3D*

ChemFinder/Word
Searching Word, Excel & More
- Searches documents for embedded structures
- Indexes structures and source locations
- Searches specified folders and whole hard drives

ChemDraw/Excel
Searching & Calculating in Excel
- Displays *ChemDraw* structures in spreadsheet cells
- Adds chemical calculations to Excel functions
- Useful for graphing and analyzing chemical data

Purchase/Excel
High Throughput Purchasing
- Finds vendor and price information from *ChemACX Database or ChemACX.Com*
- Search for suppliers and purchase online
- Maintains lists of compounds

CombiChem/Excel
Combinatorial Chemistry in Excel
- Generate combinatorial libraries
- Choose starting materials and reaction schemes
- View structures and track plate/well assignments

SYSTEMS & LANGUAGES

English & Japanese
Windows: 95, 98, Me, NT, 2000, XP
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CS ChemInfo

Reference and Chemical Databases

The Merck Index is an encyclopedia of chemicals, drugs, and biologicals, with over 10,000 monographs covering names, synonyms, physical properties, preparations, patents, literature references, therapeutic uses and more.

ChemACX Pro includes 500,000 chemical products from 300 supplier catalogs, searchable with a single query by structure, substructure, name, synonym, partial name, and other text and numeric criteria. *ChemACX-SC* is a compilation of searchable catalogs from leading screening compound suppliers.

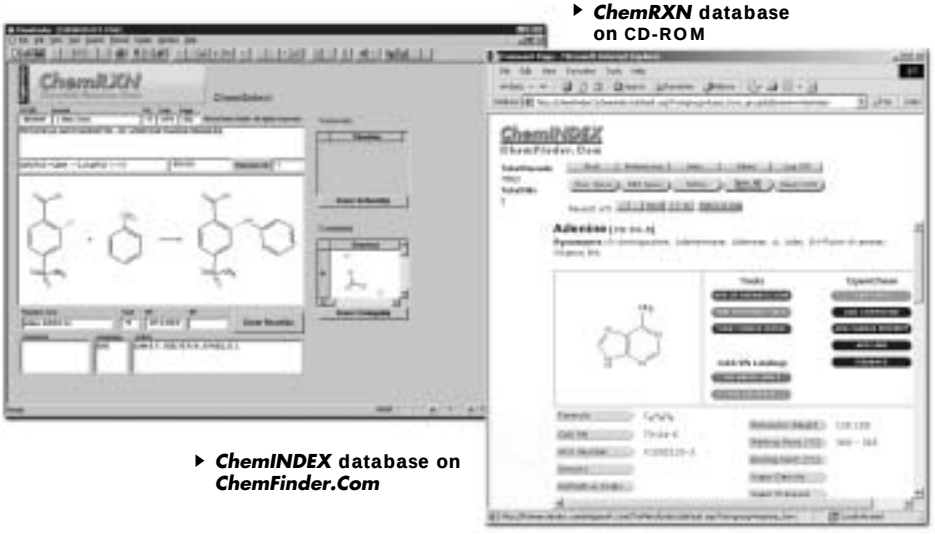
ChemACX.Com is the *ChemACX* web site with full search capabilities and convenient online ordering from major suppliers.

ChemINDEX includes 100,000 chemicals, public NCI compounds, and more.

ChemRXN is a collection of 30,000 fully atom-mapped reactions selected and refined from the chemical literature. It includes reactions from InfoChem's ChemSelect database and ISI's ChemPrep database.

ChemMSDX provides material safety data sheets for 7,000 pure compounds.

ChemFinder.Com is the award-winning web site with information and WWW links for over 100,000 chemicals. Search by name or partial name, view structure drawings, or use the *ChemDraw Plugin* for structure and substructure searches. View live *ChemDraw* files on Windows and Macintosh clients.



▸ ***ChemRXN*** **database on CD-ROM**

▸ ***ChemINDEX*** **database on *ChemFinder.Com***

SOFTWARE

The Merck Index
- Encyclopedic chemical reference

ChemACX Pro
- Chemical searching & buying

The Merck Index
Chemistry's Constant Companion
- Over 10,000 monographs of chemicals, drugs & biologicals

ChemACX Pro
Chemical Searching & Buying
- Database of commercially available chemicals: 300 catalogs with 500,000 chemical products
- *ChemACX-SC* database with 500,000 structures from leading screening compound suppliers

ChemACX.Com
WWW Chemical Searching & Buying
- Search by text, structure or substructure and order online from major catalogs

ChemINDEX
Reference Searching & Information
- NCI database of over 200,000 molecules, with anti-HIV & anti-cancer assay data

ChemRXN
Reaction Searching & Information
- Includes ChemSelect with reactions from InfoChem GmbH & ISI's ChemPrep

ChemMSDX
Safety Data Searching & Information
- Provides full Material Safety Data Sheets for over 7,000 pure compounds

ChemFinder.Com
WWW Reference Searching & Info
- WWW links for over 100,000 compounds
- Enter text queries or use *ChemDraw Plugin* for structure & substructure searching
- Works with Netscape & MS Internet Explorer

SYSTEMS & LANGUAGES

English & Japanese
Windows: 95, 98, Me, NT, 2000, XP
CD-ROM software is Windows only.
All specifications subject to change without notice.

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ChemOffice WebServer

Enterprise Solutions, Applications and Databases

ChemOffice WebServer

ChemOffice WebServer is the leading solution platform for enterprise, corporate intranet, and Internet scientific information applications. Compatible with major databases including Oracle, SQL Server, and Microsoft Access, *ChemOffice WebServer* is the development and deployment platform for custom applications and those listed below.

ChemOffice Browser

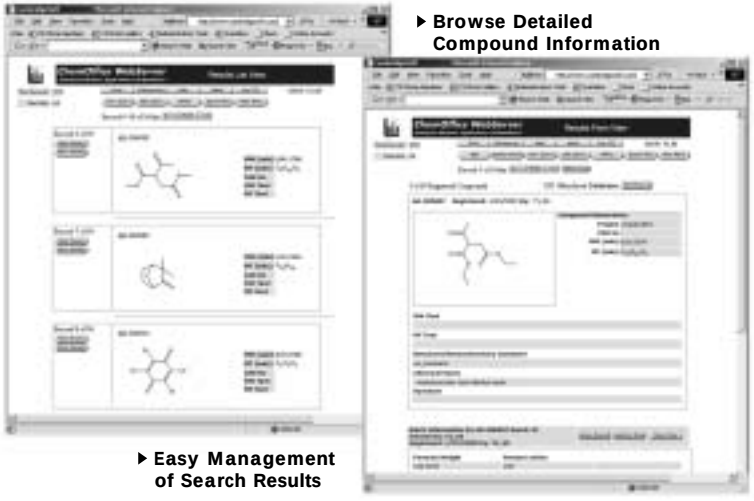
ChemOffice Browser, including *ChemDraw* Java, ActiveX, and the *ChemDraw* and *Chem3D Plugins*, brings the power and chemical intelligence of *ChemOffice* to Internet and intranet applications.

User Friendly & IT Ready

User-friendly and IT ready *ChemOffice WebServer* and *Browser* enterprise solutions, applications and databases are easier and faster for users to learn and the IT staff to deploy. Using *ChemOffice WebServer* technology, along with familiar browser technology, overall costs are lowered and less time is required for implementation.

Enterprise Solutions

Enterprise solutions built upon *ChemOffice WebServer,* including *Oracle Cartridge*, help workgroups and organizations collaborate and share information, just as *ChemOffice* supports the daily work of the scientist.



▸ **Browse Detailed Compound Information**

▸ **Easy Management of Search Results**

SOLUTIONS

- Development and deployment platform for workgroup and enterprise chemical information applications
- Webserver and browser components facilitate application deployment to desktops with minimal impact and training
- Enterprise Solution applications address areas of Knowledge Management, Research & Discovery, Applied BioInformatics and Chemical Databases

Knowledge Management

Knowledge Management applications organize and distribute chemical information. *E-Notebook Enterprise* streamlines daily record keeping with rigorous security and efficient archiving, and facilitates information retrieval by structure and text searching. *Document Manager* indexes the chemical structure content of documents, *Discovery LIMS* tracks laboratory requests, and *21CFR11 Compliance* implements an organization's regulatory compliance processes.

Research & Discovery

Research and discovery applications include *Registration System* for managing proprietary compound information, *Inventory Manager* for reagent tracking needs, and chemical databases for complete management of chemical inventories. *Formulations & Mixtures* and *CombiChem Enterprise* also provide tailored approaches to managing chemical data.

Applied BioInformatics

BioAssay HTS and *BioSAR Browser* applications process biological assay data to pinpoint the structural determinants of biological activity. *BioAssay HTS* supports low, high, and ultra-high throughput workflow, including sample and plate management, while *BioSAR Browser* probes structural details within assay data.

Chemical Databases

The Merck Index and *ChemACX Database* provide reference information, property estimations, and searchable compilations of commercially available chemicals.

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Oracle Cartridge

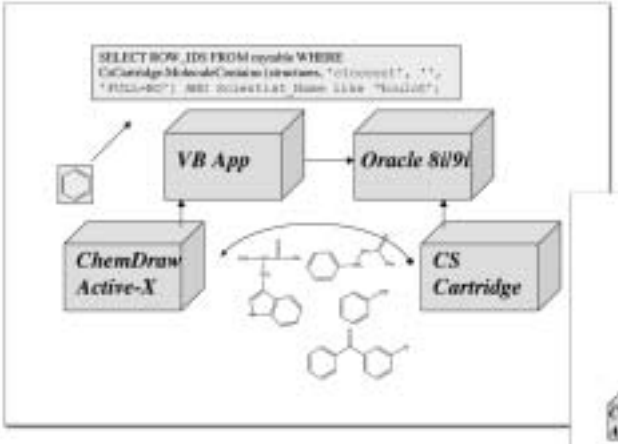
Enterprise Infrastructure for Database Security

WebServer Oracle Cartridge

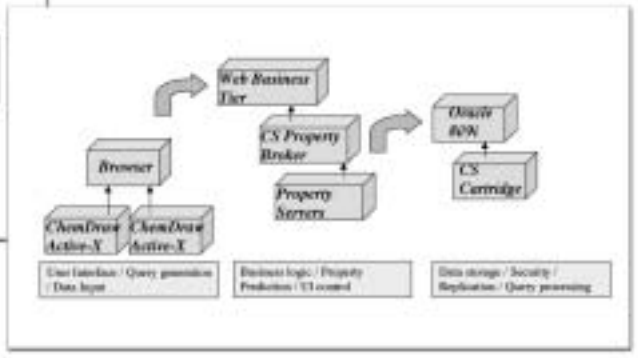
In scientific applications, the ability to store and manipulate chemical information is essential. By using CambridgeSoft's *Oracle Cartridge*, you add chemical knowledge to your Oracle platform and automatically take advantage of Oracle's security, scalability, and replication without any other external software or programs. You can search the chemical data by structure, substructure, and similarity, including options for stereo-selectivity, all through extensions to Oracle's native SQL language. Tools like PowerBuilder, Visual Basic and Visual C++ readily lend themselves as database clients. With the addition of the *ChemDraw* ActiveX control in the client, your end users can be structure-searching in no time.

Chemical Data Formats

CambridgeSoft recognizes that there is an enormous amount of legacy data out there in a myriad of formats, and most users have no desire to make wholesale changes to their chemical data generation or storage. To this end, *Oracle Cartridge* supports all major data types without translation or modification. In addition to CDX, it supports CDXML, MolFile, Rxn, and SMILES formats. Moreover, there are built-in extensions to SQL that allow you to extract data in all supported formats. Due to the variety of data formats supported, *Oracle Cartridge* is easily deployed even within existing applications. Since no manipulation of the data is needed, new records are automatically added to the index for searching.



▸ **Simple Client-Server Architecture**



▸ **Web Based Architecture**

- Adds chemical data types to Oracle, linking chemical applications to enterprise software systems without special programming
- Confers Oracle's security and scalability, simplifying large-systems' architectural considerations
- Makes legacy chemical data, such as MDL ISIS, accessible to *ChemOffice WebServer* applications

WebServer Enterprise Solutions

Even if you're not developing your own applications, or interested in the advanced data portability aspects of the *Oracle Cartridge*, CambridgeSoft's strategy will have a positive benefit for your IT infrastructure. CambridgeSoft's enterprise solutions are available in *Oracle Cartridge* versions, including *E-Notebook Enterprise*, *Document Manager, Registration System*, *Inventory Manager*, and *BioAssay HTS*. By utilizing *Oracle Cartridge*, you can deal with issues such as scalability and security entirely through the database layer, simplifying large-systems' architectural considerations. *Oracle Cartridge* has the side benefit of providing a database-level interface to key applications, so developers can integrate CambridgeSoft's solution platform with in-house IT solutions without tinkering with the business tier. Communicating with *Oracle Cartridge* is as simple as learning a few extensions to SQL.

Systems & Support

Support extends to include a variety of UNIX operating systems in addition to Windows servers. *Oracle Cartridge* has been deployed by large pharmaceutical companies with Oracle 8i and 9i.

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E-Notebook Enterprise

Desktop to Enterprise Knowledge Management

E-Notebook

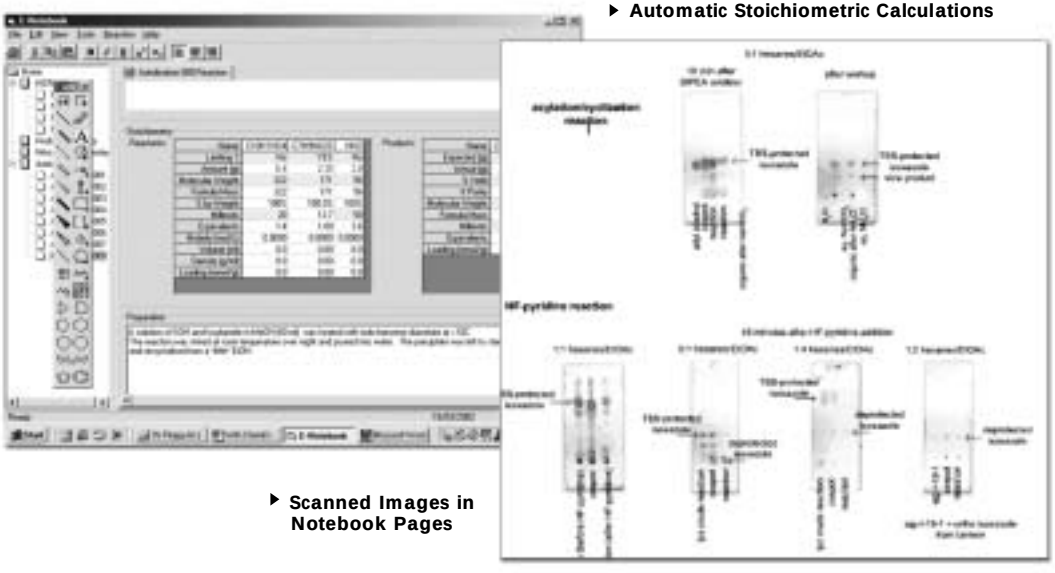
E-Notebook provides a smooth web-based interface designed to replace paper laboratory notebooks, with a fully configurable, secure system for organizing the flow of information generated by your organization. You can enter reactions, Microsoft Word documents, spectra and other types of data, and then search this data by text, substructure or meta-data. You can organize your electronic pages by projects, experiments or any other classification that conforms to your workflow.

Desktop to Enterprise

E-Notebook allows organization of notebook pages at either the personal or enterprise level. Enterprise groups can organize and store notebook pages in a central data repository, allowing colleagues to take advantage of each other's work. All access to data is subject to granular security. *E-Notebook* works with *Oracle Cartridge* and SQL Server, for departments or entire enterprises, and Microsoft Access, for individuals or small groups.

ChemDraw & Stoichiometry Calculations

While not quantum theory, stoichiometric calculations remain long and tedious. *E-Notebook* tackles this troublesome problem. First, draw your reaction directly in the page. Then, simply enter the mass, volume and den-



▸ Automatic Stoichiometric Calculations

▸ Scanned Images in Notebook Pages

- Custom organization of notebook pages at personal or enterprise levels with links to chemical registration
- Notebook pages include *ChemDraw* reaction schemes, Microsoft Word and Excel documents, and spectral data using the Galactic Spectral Control
- *Oracle Cartridge* provides detailed security and data integrity; SQL Server also available

sity, volume and molarity, and other factors of the limiting reagent and specify the number of equivalents of the other reactants. The notebook will do everything except calculate the experimental yield. To do that, you still have to run the experiment!

Microsoft Office & Galactic Spectra

E-Notebook manages all the other kinds of data chemists store in their notebooks. For free-form data, you can include Microsoft Word or Excel documents. For spectral data, you can take advantage of the Galactic Spectral Control embedded in the notebook that allows for analysis and storage of hundreds of kinds of spectra files.

Inventory Manager

E-Notebook includes an inventory of common reactants and reagents. If you have one of these common components loaded into the inventory application, all you have to do is click the *Add Reactant* button in *E-Notebook*. From here, you navigate to the desired compound and include it in your stoichiometry calculations. The enterprise edition of *E-Notebook* integrates with procurement and inventory management systems. Not only does this provide a useful way to know what compounds you have in stock and where they are located, it also saves time entering data.

Registration System

E-Notebook can be integrated into the entire chemical workflow of enterprise organizations. For example, once you record a reaction in your notebook, you can click a button to forward the products of the reaction to your compound registration system. These kinds of workflow enhancements increase productivity for the entire organization.

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Document Manager

Desktop to Enterprise Document Searching

Document Manager

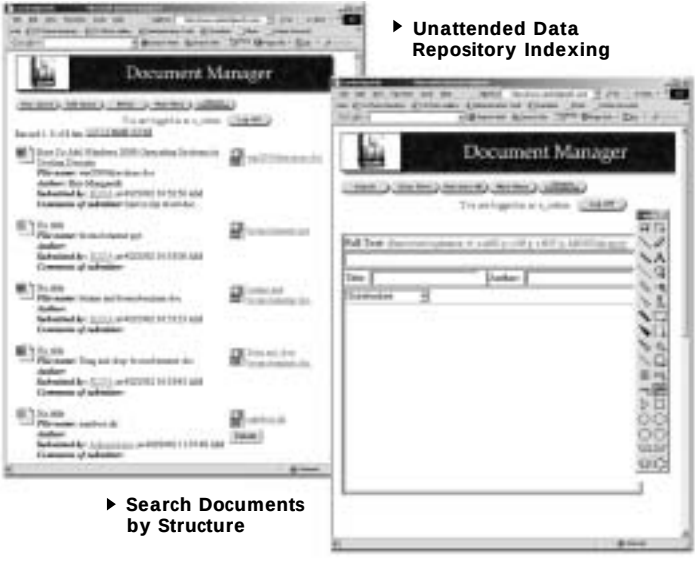
Everyone produces reports electronically, but searching information located in these reports has always been difficult. Thousands of Microsoft Word, Excel, PowerPoint, and other documents reside on file servers or individual computers, with no way to globally search them for information. Certainly, no easy way exists to search for the chemistry contained in these documents. *Document Manager* solves this problem, and requires no change in how you write and distribute reports.

Easy to Use

Document Manager manages a repository of new documents. These can be Microsoft Word, Excel, PowerPoint, or many other document types. When a new document is added, *Document Manager* automatically builds a free-text index of the document, and automatically extracts the chemical information into a chemically-aware, substructure searchable database. Chemical information can be both *ChemDraw* and ISIS/Draw. Finding information in reports is now as simple as entering a query through your web browser.

Unattended Data Indexing

As new documents are added they are automatically indexed and chemical information is extracted. Similarly, if a document is modified, it is re-indexed. No administration of the server is necessary other than routine back-up.



▸ **Unattended Data Repository Indexing**

▸ **Search Documents by Structure**

MANAGEMENT

- Indexes chemical structure information in documents and compiles a structure-searchable database
- Monitors designated folders or drives and automatically indexes new documents as they appear
- Documents are searchable by structure and free text

Free Text Searching

Documents are searchable by free text, including Boolean expressions, proximity operators, or simple queries. For example “author near Saunders” finds all Word documents where the word “author” appears near the word “Saunders”.

Advanced Chemical Searching

Since the chemical information is automatically extracted, documents can be queried by structure, substructure, similarity, molecular weight and formula. Chemical queries also support atom lists, Boolean operations on structures, superatoms, functional groups and many others. Queries can also be refined after an initial search, extending the power of the query language.

Structured Document Support

Structured documents, including documents created with Word templates or XML, are also supported. Information in structured documents is extracted and stored in specific fields of the database for more precise searching.

ChemFinder/Word

ChemFinder/Word, the desktop version, searches Word documents, Excel spreadsheets, *ChemDraw* files, *ChemFinder* databases, SD files, MDL molfiles, and more. Unlike other Microsoft Find facilities, *ChemFinder/Word* lets you work with the results you’ve located. Once you have a hit list, you can browse, search, refine, or export it to any destination.

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21CFR11 Compliance

Electronic Records and Signatures Regulations

The Challenge

Large and growing enterprises are facing a challenge to their core missions of developing and producing new products including food, therapeutic pharmaceuticals, medical devices, cosmetics or other health enhancing items. The complexity lies in complying with government regulations designed to protect public health and safety. The most notable of these is Title 21 of the Code of Federal Regulations governing Electronic Records and Signatures (21CFR11). Although 21CFR11 has been in the draft stage for almost a decade, final regulations have recently been created. Enforcement of these regulations is beginning to take place and enterprises are responding with a wide variety of initiatives, both within individual organizations and across industry sectors.

Integrated Software

CambridgeSoft applications, such as *E-Notebook Enterprise* and *Document Manager*, are at the leading edge of the integration of corporate knowledge management with *21CFR11 Compliance*. These products are designed so that as your organization reviews its internal processes for *21CFR11 Compliance*, the software can be configured to support these internal processes. Major requirements of 21CFR11, such as electronic signatures, audit trails, and long-term archiving, are incorporated within the routine workflow to generate the critical information required by research, development and production. In addition, *E-Notebook Enterprise* and *Document Manager* can be integrated with existing critical data systems.

▸ **Document and Record Management**

▸ ***E-Notebook* Data Capture**

- *E-Notebook Enterprise* and *Document Manager* integrate corporate knowledge with regulatory compliance
- Consulting teams analyze and adapt existing procedures to comply with new regulations
- Systems include authentication and digital signatures and adapt to changing regulations and demands

Analysis

As your enterprise develops the operating procedures that you will need to adopt for *21CFR11 Compliance*, CambridgeSoft's consulting team can provide invaluable assistance in analyzing your current operating procedures, adapting your existing procedures to comply with new regulations, and validating the software and the operating procedures that you will use. CambridgeSoft's consulting teams consist of individuals who have extended experience in deploying systems used by large pharmaceutical companies, emerging biotechs, and major enterprises worldwide.

Implementation

Once you have determined how your enterprise will comply with these new regulations, implementing those decisions needs to be done quickly, efficiently and with the understanding that the rules for compliance are in flux. In order to succeed, you must be able to respond to change. CambridgeSoft's *21CFR11 Compliance* consulting has both the tools and the expertise to provide complete solutions, carry out integration with your existing systems, and help you execute the process as quickly as your organization demands. Since ongoing monitoring is a part of business for regulated industries, you can be confident that, as regulations evolve and your requirements change, your systems can adapt. With CambridgeSoft, you can take advantage of the knowledge that has helped dozens of businesses, large and small, gain control over their business processes, their intellectual capital, and their material resources.

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Registration System

Chemical and Biological Registration

Registration System

Registration System includes a robust data model for pure compounds, batches, salt management, automatic duplicate checking and unique ID assignments. Compounds may be entered individually or with SD files. The data model resides entirely in Oracle and uses Oracle's security and transaction framework. For companies intending to modify or construct their own registration system, *ChemOffice WebServer* includes a powerful Software Developer's Kit (SDK) to add custom functionality. Instead of inventing a proprietary language, *ChemOffice WebServer* SDK extends the Microsoft and Oracle platforms, allowing information scientists to use the industry's most powerful development tools.

ChemDraw Plugin & WebServer

Registration System is easily adapted in almost any work environment. Its web-based, industry standard *ChemDraw* interface, makes *ChemOffice WebServer* the best choice for your corporate scientific information.

User Friendly Chemical Registration

New compounds are entered through a web form, and chemical, along with non-chemical, data is kept in a temporary storage area. When the compound is registered, it is compared for uniqueness via a configurable, stereoselective duplicate check, and assigned a registry number. All information about the compound, including its test data and other syntheses, is tracked by the registry number.

▸ Search for a Compound

▸ Display & Format Results

- Accessed through your favorite web browser, the system uses Oracle with robust data model to manage chemical products and their properties
- Checks for uniqueness during registration and optionally registers duplicates as batches of existing substance
- User administration and data entry are done through simple, easy-to-learn web forms; highly configurable system avoids tedious and expensive customization

Duplicate Checking with Override

When compounds are registered, the structure is checked for novelty. If a duplicate already exists in the database, the user can elect to register the information as a new batch of the existing compound, or assign it a unique registry number.

Oracle Cartridge

Registration System is the only true n-tiered application of its kind that is designed around thin clients and thin servers. This translates into ultimate flexibility on both the client and server side. Oracle is supported as a host, both with native security, on a variety of platforms and operating systems. The chemical information is directly stored in the Oracle tables.

Web Based User Interface

While the business logic of *Registration System* is complex, its user interface is clean and simple. Web browser support for Netscape Navigator and Internet Explorer, plus a choice of *ChemDraw Plugin*, *ActiveX* or *Java* client tools are provided. This significantly reduces training time and cost of client maintenance.

Advanced Chemistry Features

Duplicate checking is stereochemically aware. Batch data is maintained separately from compound data. Registration numbers support multiple sequences, including one for synthesized and one for procured. Compounds can be tracked by project and notebook reference, and registered in batches from SD files or other sources of molecular information.

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Inventory Manager

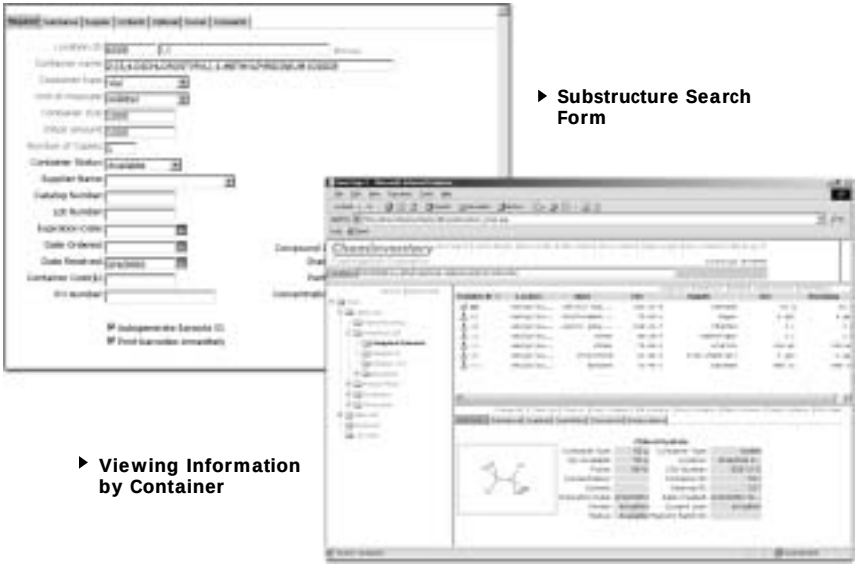
Chemical and Biological Inventory Integration

Database Technology

Inventory Manager is a *ChemOffice WebServer* based application designed to manage the reagent tracking needs of chemical and pharmaceutical research centers. The system manages data associated with both commercially and internally produced chemical substances. Although *Inventory Manager* is a stand-alone application, it can be tightly integrated with CambridgeSoft's *Registration System* and chemical procurement *ChemACX Database*. *Inventory Manager* is designed for a range of sizes from large workgroups to enterprises, and captures both stockroom and reagent needs as well as high-throughput discovery.

Cascading Location Model

Inventory Manager has a fully cascading location model. This means that laboratories can decide for themselves the granularity of their locations. Some labs may define locations as wells on plates residing on shelves inside refrigerators, which, in turn, are found in laboratories. Another lab may decide to track reagents at the bench or cabinet level. Still, in other settings, it may suffice to track chemicals on a lab-by-lab basis. The moving of chemical inventories is greatly helped by this model. For example, if an entire refrigerator is relocated, all of its containers move along with it. There is no need to re-catalog or reconcile, which saves a great deal of time.



▸ **Substructure Search Form**

▸ **Viewing Information by Container**

- Integrated with *Registration System* and *ChemACX* for procurement and life cycle chemical tracking
- Cascading location model allows different labs to track reagents at different levels (stockroom, refrigerators)
- Designed for tracking reagents, high-throughput discovery libraries, and true HTS plate management at multiple levels

Discovery, Reagents & Stockroom

Inventory Manager integrates fully with CambridgeSoft's *ChemACX Database* of available chemicals and *Registration System*. It also functions completely as a stand-alone application. Through this architecture, CambridgeSoft's enterprise solutions are truly plug-and-play. There are no added system integration costs, and the applications can live on different servers in different parts of the world.

Flexibility

The flexibility of the location model allows *Inventory Manager* to accommodate both reagent and discovery inventories in the same system. Each container in the system can be configured to track quantities in increasingly small values. A reagent bottle, for instance, can be measured as "full" or "empty", while wells in a 96-well plate can be measured in microliters. By moving such settings and preferences down to the container level, rather than system-wide or custom programming, *Inventory Manager* can accommodate both worlds in a single instance.

Integration with Purchasing & Registration

Inventory records are created directly from *ChemACX Database* of available chemicals, as well as from *Registration System*. For substances that do not exist in either database, *Inventory Manager* has its own chemically aware user interface. By tightly coupling with *ChemACX Database* and *Registration System*, the need for duplicate data entry is virtually eliminated. Once a product is ordered, its chemical information is stored and it is given an "on order" status, reducing duplicate ordering of popular reagents.

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CombiChem Enterprise

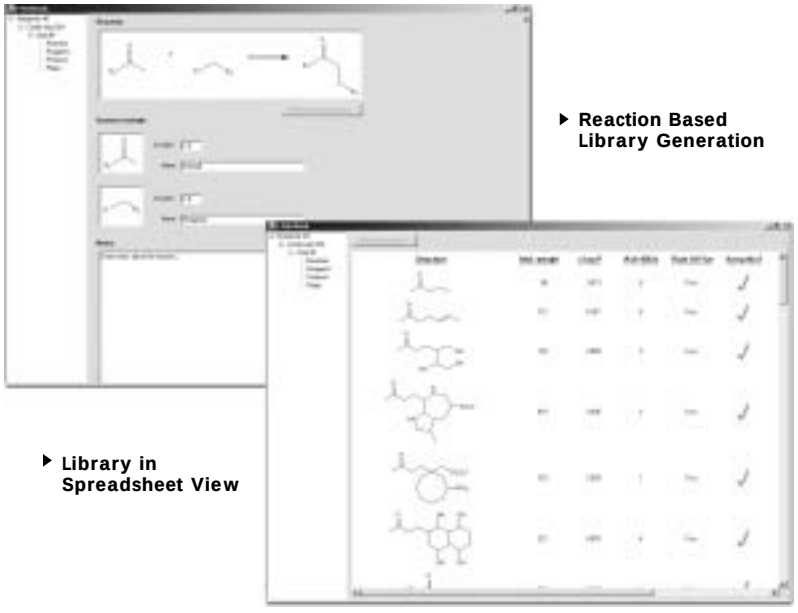
Desktop to Enterprise Combinatorial Chemistry

Benefits of Combinatorial Chemistry

Combinatorial chemistry, in particular the technique of parallel synthesis, has become an essential element of the drug discovery process. This is true both at the point of finding new leads as well as optimizing a promising lead. By using parallel synthesis techniques, chemists are able to multiply their productivity by a factor of between 5 and 100. This increase in productivity creates data management challenges. *CombiChem Enterprise* has been developed to provide the software tools required by the combinatorial chemist to manage and document parallel synthesis experiments. The software models real-world workflow as much as possible.

Starting Out

To start, the user simply draws a generic reaction step in a *ChemDraw* ActiveX control directly embedded in the notebook environment. Multiple reactants and products are supported. Points of variability on the molecules are indicated by the traditional "R" designation. Furthermore, query features can be used to precisely define the intended molecules. After drawing the reaction, the software analyzes the generic reaction, determines the role of each molecule, and creates pages for managing the lists of real reagents to be used in the actual parallel synthesis experiment.



▸ **Reaction Based Library Generation**

▸ **Library in Spreadsheet View**

- Reagent lists can be drawn from varied sources
- Reaction based library generation allows for evaluation by product or reagent
- Data management is simplified and library specifications are available to others on the network

Finding Reagents

Flexibility is the key when dealing with databases of chemical compounds. *CombiChem Enterprise* can use reagent lists from a variety of different sources: SD files, *ChemFinder* databases, *ChemFinder* hit lists, *ChemOffice WebServer* hit lists, *ChemACX Database*, or directly from the user via *ChemDraw*. Regardless of the source, *CombiChem Enterprise* produces a list of reagents which match a particular generic reactant. The chemist then chooses which of the compounds to use for generating products.

Getting Results

Once the chemist has given *CombiChem Enterprise* a set of reagents for each of the generic reactants in the reaction scheme, the software generates the set of products which would result from running the experiment. *CombiChem Enterprise* evaluates the products using several *in silico* methods, and the chemist can then choose which compounds to keep and which ones to reject. After the products have been generated, the software provides product information for each of the reagents. The chemist can use that information, for example, to trim away reagents having few or no products which pass the Lipinski Rule of Five test. Finally, the products are laid out on plates based on user-definable plate layouts.

Integration with *E-Notebook*

Keeping track of compound library data can be a challenge: which reagents led to this product, which product goes with that spectrum, what was in the mixture used in this thin layer chromatography? *CombiChem Enterprise* provides ways to organize the data and navigation is simple. When used with *E-Notebook Enterprise*, the data for a library of shared compounds, and the entire experiment, is automatically documented and made available to the entire organization.

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BioAssay HTS

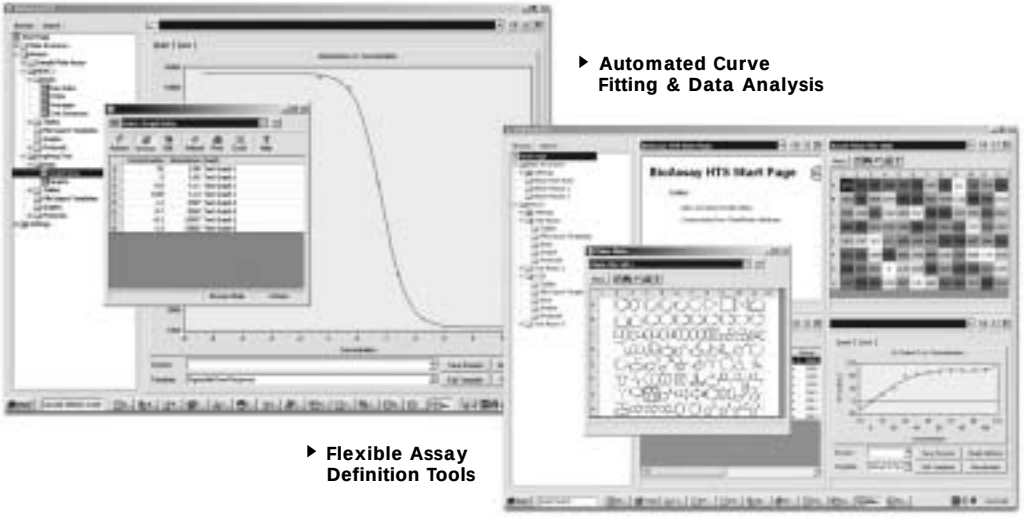
Biological Assay and High Throughput Screening

BioAssay HTS

BioAssay HTS provides scientists with an effective way of managing test results for biological and other kinds of experiments intended to assess the efficacy of compounds. Suitable for both plate-based high throughput screening assays and smaller-scale lead optimization experiments, *BioAssay HTS* provides researchers with simple tools for setting up their models in a database, uploading data, automating calculations and reporting on their findings.

User Friendly Assay Management

Even for the most basic protein assays, the independent and dependent variables used by the biologist to quantify efficacy can vary substantially from assay to assay. The underlying requirement that follows from this variability is for a flexible data management system that can adapt quickly to different assays and biological models. With *BioAssay HTS*, researchers or IT support staff simply define the observables and calculations that make up the assay. The database does the rest. Users can set up unlimited levels of drill-down. This allows users, for example, to click an IC50 and see a graph of percent inhibition versus concentration. Click again, and the software displays the original triplicate results, with outliers marked. The software even supports complex *in vivo* models.



- Effectively manages data from complex biological assays involved with lead optimization
- Adapts quickly and flexibly to different assays and biological models
- Closely integrated with Microsoft Excel, *ChemOffice* and *ChemDraw*

Easily Manage Large Volumes of Data

BioAssay HTS offers an easy way to capture large volumes of data from automated laboratory equipment and store it securely in Oracle. Scheduled data import means you can set up an import template once, and all future data will appear in the system as it is gathered. *BioAssay HTS* contains a complete plate inventory system that tracks plates and compound groups across plates. It easily manages daughter plate creation, barcoding, and freeze/thaw cycle tracking. Since it is integrated with your assay data, you can instantly view compound information and visualize results plate-wise to detect anomalies before they become a problem.

Automated Calculations & Curve Fitting

Once the database is configured for an assay, calculations are performed automatically whenever new data is entered or imported. Calculations can be quite complex, built from multi-step procedures. For an IC50 assay in triplicate, the software can average your triplicate results, take control values into account, and perform a sigmoidal dose-response curve fit according to your specifications. It is now as easy to do for 10,000 compounds as it is for ten.

Find Structure-Activity Relationships

Users can visualize data for multiple assays with *BioSAR Browser*, which is specifically designed for viewing structures and alphanumerics side-by-side. Other components of the *ChemOffice* product line provide additional ways to analyze structural and biological data and perform structure searches. Both *ChemFinder* and *ChemOffice WebServer* make it easy to create customized forms for viewing data. Users can export data to Excel or Spotfire for further analysis and reporting.

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BioSAR Browser

Biological and Chemical Meta Data Catalog

BioSAR Browser

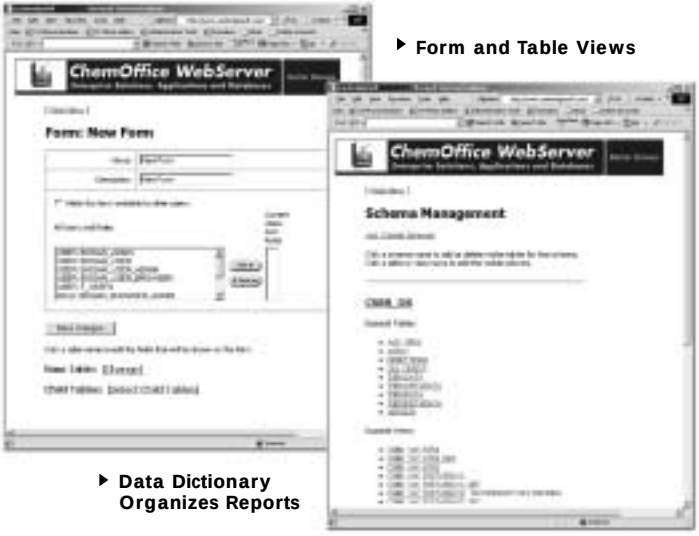
BioSAR Browser, a strategic must for any discovery organization interested in serious data mining, is a data-dictionary driven structure-activity analysis program. Users may choose among assays registered in the dictionary or search for assays of interest.

Providing Catalog Capabilities

The power of *BioSAR Browser* lies in the researcher's freedom from dependence on IT support. Once an assay is registered into the data-dictionary it is automatically included in the powerful analysis framework. By reducing the time between question and answer, *BioSAR Browser* gives researchers the freedom to explore new ideas—the bottom line for discovery information systems. Systems that provide answers after questions have become irrelevant are of no use. *BioSAR Browser* avoids this by placing application development in the researcher's control.

Forms & Tables in a Unified Interface

While most SAR tools provide only a table-based interface, *BioSAR Browser* provides a forms-based interface in addition to a tabular view. Researchers have demonstrated that both form and tabular views are essential. Forms provide highly detailed information about one compound, whereas tabular views make comparisons between



▸ **Form and Table Views**

▸ **Data Dictionary Organizes Reports**

- Catalog driven data mining and analysis operation
- Both form and table views available within simple web interface; *ChemDraw for Spotfire*
- Role based security specifies operations allowed for administrators, publishers and browsers

compounds more feasible. There is often a tradeoff between power and simplicity, and most SAR tools opt for the former at the expense of the latter. *BioSAR Browser*, however, merges the sophistication of a powerful data catalog technique with knowledge gained through years of working closely with users. The result is a SAR application that is as intuitive as it is powerful.

Security & Convenience

Security within *BioSAR Browser* is highly granular. Different roles exist for administrators, publishers, and browsers. Administrators may add assays to the data catalog engine, publishers may create reports and publish them, and browsers may use data query and analysis. Most data mining tools provide a mechanism to store queries, but the interface for creating queries is too complex. With *BioSAR Browser*, each set of assays is a complete report with a query form, a view form, and a table view, combining the convenience of a *ChemFinder* or ISIS application with the power and flexibility of a data catalog-driven mining program.

ChemDraw for Spotfire

ChemDraw for Spotfire is a powerful add-in for the Spotfire DecisionSite software. Spotfire makes industry standard applications for high-dimensional visual data analysis, and is used to explore large biological datasets. *ChemDraw for Spotfire* adds chemistry to DecisionSite, providing structure visualization and searching services. Highlight a spot in Spotfire's DecisionSite, and a structure is displayed directly in the window. If you draw a structure and click *Search*, the matching records are displayed right in the Spotfire window. The structures are retrieved from a chemical database such as *Registration System*, *ChemFinder*, or *Oracle Cartridge*, and are returned directly over the network. In this way, structures can be linked by registry number, CAS number, or

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ChemACX Database

Available Chemicals and Screening Compounds

ChemACX Database

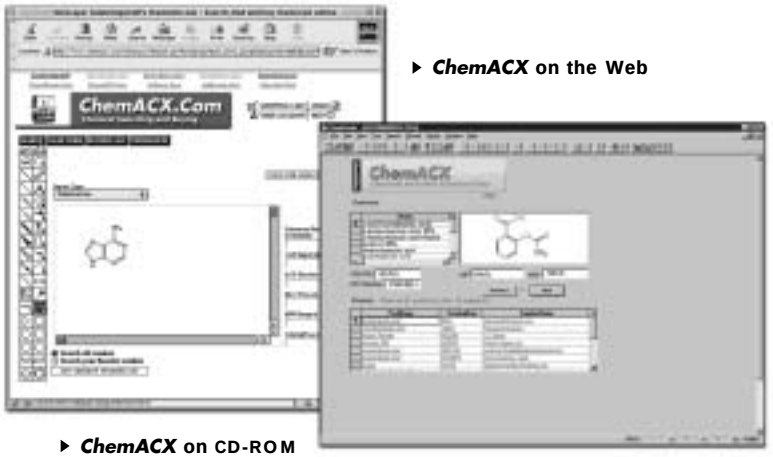
Sifting through chemical catalogs is a poor use of time for any researcher. The Available Chemicals Xchange database, *ChemACX Database*, provides a complete tool for research chemical sourcing and purchasing. The database can be accessed from both desktop and enterprise environments and boasts an impressive list of major suppliers, from Alfa Aesar and Aldrich, to TCI and Zeneca with hundreds in between. The enterprise procurement solution for *ChemACX* saves time by streamlining the entire purchasing process. Use *ChemACX* to build an internal requisition, print the form on your company template, fill it out and submit it to purchasing.

ChemACX-SC

ChemACX-SC is an additional fully structure searchable database containing the catalogs of leading screening compound suppliers, including ChemBridge, Maybridge, Sigma-Aldrich's Rare Chemical Library and others.

Data Quality

Over 500,000 products from 300 research chemical and biological catalogs have been selected to have their product catalogs prepared for electronic delivery. The data provided by the suppliers is enriched by editors who add searchable chemical structures, physical and chemical properties, and incorporate a comprehensive chemical synonym dictionary. All substances and supplier catalog numbers are cross-referenced, making it easy to locate alternate sources for back ordered or discontinued items.



▸ ***ChemACX* on the Web**

▸ ***ChemACX* on CD-ROM**

- Fully structure-searchable database of 500,000 products from 300 chemical catalogs; separate *ChemACX-SC* database contains screening compounds
- Search by name, synonym, partial name, formula, and other criteria, as well as structure and substructure
- Shopping cart system works with requisition forms and purchasing systems, such as SAP, Ariba and Commerce1, to streamline chemical purchasing

Data Currency

A premium is placed on the accuracy and currency of the *ChemACX Database*. Many suppliers listed in the database are also currently selling their products online through the *ChemACX.Com* web site, and therefore have a vested interest in ensuring that their data remains complete, accurate and up-to-date. You won't find a sourcing database with more frequently updated content and current pricing than *ChemACX*.

Data Accessibility

The same way that Internet users can publicly access *ChemACX.Com*, enterprise users can access their private *ChemACX Database* via a standard web browser. There is no need to configure or install any additional software. *ChemDraw* users can either use the *ChemDraw Plugin* to draw chemical structures directly in the browser's search page, or alternatively submit queries to the database server directly from *ChemDraw*. *ChemFinder* users can access their own copy of the database right from their local hard drive.

Electronic Requisitions

Traditional sourcing databases were conceived merely as reference tools. *ChemACX Database*, however, goes one step further by including the ability to collect products into an electronic shopping cart and export its contents into electronic requisition forms or purchasing systems. This time-saving feature has proven to be one of the most popular advantages of *ChemACX* among scientists and purchasing agents alike. Users can readily export data from the shopping cart into Excel and Word templates used as departmental requisition forms.

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The Merck Index

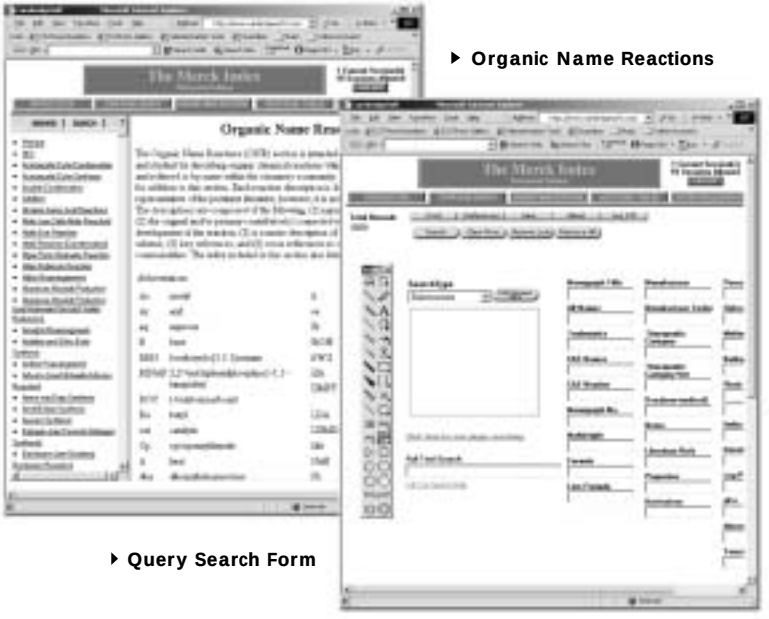
Chemistry's Constant Companion

Industry Standard

Among printed chemical reference works, one that stands out for its integrity, detail and longevity is *The Merck Index*. This encyclopedia of chemicals, drugs and biologicals has 10,250 monographs, 446 named reactions and 23 additional tables. Merck & Co., Inc., the publisher of *The Merck Index*, has chosen CambridgeSoft to produce the complete contents of the 13th edition in a fully searchable *ChemOffice* format.

Detailed Monographs

The subjects covered include human and veterinary drugs, biologicals and natural products, agricultural chemicals, industrial and laboratory chemicals, and environmentally significant compounds. What makes *The Merck Index* so valuable is its extensive coverage. The information provided includes chemical, common and generic names, trademarks, CAS registry numbers, molecular formulas and weights, physical and toxicity data, therapeutic and commercial uses, and literature citations. In addition to the standard searches, compound monographs can now be searched by *ChemDraw* structure as well as substructure. Moving this information to the fully searchable *ChemOffice* format makes it easier and faster to search and get results. Instead of consulting the auxiliary indices and then turning to the actual monograph, all searching can be done from a single form.



▸ Organic Name Reactions

▸ Query Search Form

- Encyclopedic reference for over 10,000 chemicals, drugs, and biologicals
- Fully searchable by *ChemDraw* structure, substructure, names, partial names, synonyms and other data fields
- Available in desktop, enterprise and online formats

Integrated Information

Having *The Merck Index* in *ChemOffice* format confers another valuable benefit: integration with other information sources. For example, after locating a substance in *The Merck Index*, it is a simple matter to copy the name, structure or other data elements to search *ChemACX Database* to find out whether there are commercial suppliers of the substance. The structures could also be used as input to *Chem3D* to obtain three-dimensional models and to perform electronic structure and physical property calculations. Information can also be brought into any *ChemOffice* desktop or enterprise solution, including *ChemDraw/Excel*, *ChemFinder/Word*, *E-Notebook* and *Registration System*.

ChemOffice Formats

The Merck Index is available in two *ChemOffice* compatible formats. The desktop edition is a CD-ROM in a *ChemFinder* database format, for use by an individual researcher. The enterprise edition, designed for workgroups and larger user communities, is served by *ChemOffice WebServer* to connected users. *The Merck Index* thus adds to the growing set of reference databases served by *ChemOffice WebServer*. Just as *ChemOffice* integrates the desktop edition of *The Merck Index* with the scientist's everyday activities, the enterprise edition becomes an integral part of the applications deployed on *ChemOffice WebServer*.

Web Versions

The complete contents of *The Merck Index* are also available online through your favorite web browser. To meet your specific needs, single user subscriptions, corporate extranet subscriptions and intranet webservers are all available.

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Chemical Databases

Reference, Chemicals, Reactions, Patents and MSDS

Databases

ChemOffice WebServer provides a full range of compound and reaction databases essential for research. Databases are available at *ChemFinder.Com*, or over corporate intranets.

Reference

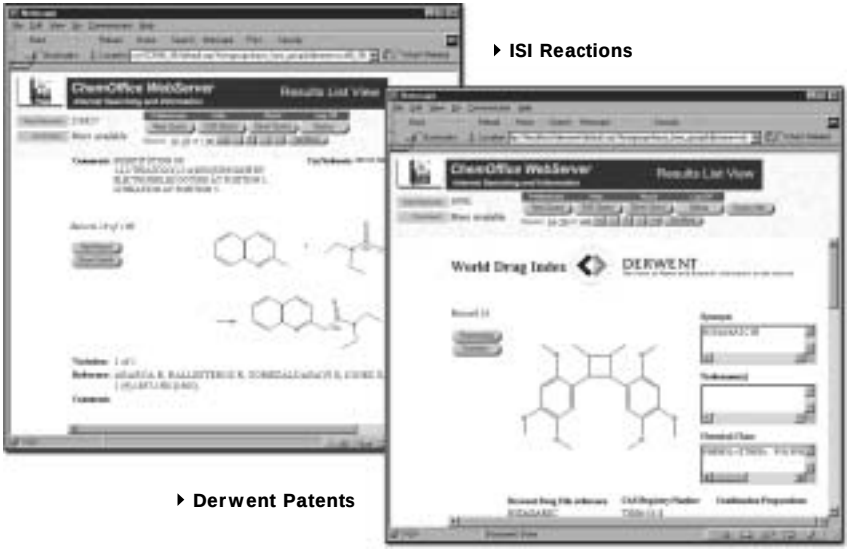
The Merck Index contains encyclopedic references for over 10,000 chemicals, drugs and biologicals.

ChemINDEX includes 100,000 chemicals, public NCI compounds and others.

World Drug Index (WDI) from Derwent contains over 58,000 compounds with known biological activity. WDI classifies compounds according to type of biological activity, mechanism, synonyms, trade names, references and more.

Chemicals

ChemACX and ***ChemACX-SC***, Available Chemicals Xchange, is a large and growing source for information on compound availability. It lists compounds from Alfa Aesar and Aldrich to TCI and Zeneca with hundreds in between, including 500,000 products from 300 catalogs. *ChemACX-SC* is a library of screening compounds.



- Extensive collection of chemical reference information in fully searchable database format
- Includes information on commercial availability; properties; biological activity; organic reactions; material safety data sheets; and patent or development status
- Developed by CambridgeSoft in partnership with the leading chemical database publishers

Reactions

Organic Syntheses is the electronic version of the annual and collective volumes of trusted, peer reviewed synthesis procedures published since 1921 by Organic Syntheses.

Current Chemical Reactions (CCR) from ISI is both a current awareness and a data mining application used to design chemical syntheses. Renowned for its quality, CCR contains information from over 300,000 articles reporting the complete synthesis of molecules. Updated daily, CCR is an excellent way to stay on top of recent developments.

ChemReact and **ChemSynth** from InfoChem are carefully selected from a database of over 2.5 million reactions through an automated process of reaction classification. With over 390,000 reaction types, ChemReact is for expert synthetic chemists designing novel syntheses. Entries in ChemSynth are further refined to those with over 50% yield and at least two literature references.

ChemRXN is a refined selection of over 29,000 fully atom-mapped reactions. Including carefully selected reactions from InfoChem's ChemSelect database and ISI's ChemPrep database, *ChemRXN* is a terrific combination of utility.

Patents

World Drug Alerts (WDA) from Derwent is a current awareness application providing information on patents, new biologically active compounds, new methods for synthesizing drugs, and other data. It is a requirement for effective decision making in all stages of drug design.

Investigational Drugs Database (ID db) from Current Drugs is the world's leading competitor intelligence service on drug R&D. Updated weekly, it covers all aspects of drug development world wide, from first patent to launch or discontinuation.

Safety MSDS

ChemMSDX provides over 7,000 material safety datasheets.

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Consulting & Services

Development, Installation & Training Services

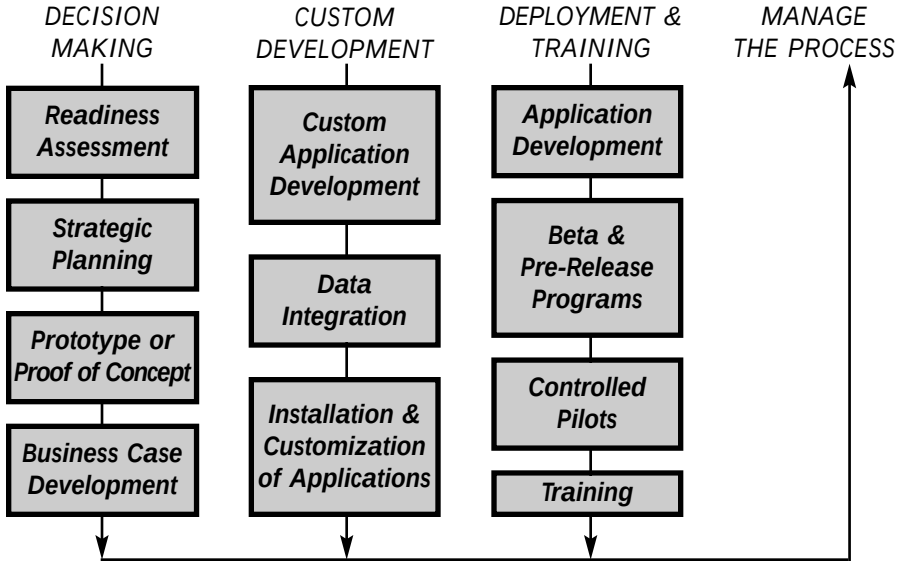
Managing Information

Today's businesses are facing many complex issues. Among them are the overloads of disparate types of information, unmanaged proliferation of valuable research data, virtual projects in many locations, uncontrolled research data, compliance, certification and regulation. Technological solutions to these issues require careful planning and management. CambridgeSoft now offers the following professional services to assist businesses in fully utilizing the power of technology.

Decision Making

CambridgeSoft believes that successful technology utilization begins with the assessment and decision making process. Our experts can assist clients with:

- *Readiness Assessment*: Identify the scope, requirements, and deliverables for your project. Assure critical IP is incorporated. Allow end-users to capitalize on existing scientific and technology resources.
- *Strategic Planning*: Conduct formal analysis of scientific, technical, operational, and process environments to determine the necessary approach to customization and deployment.
- *Prototypes and Proof of Concept*: Prototypes allow you to test the technical feasibility of solutions. This activity can provide a baseline for the future roll-out of the solution, and can also gather user feedback so requirements can be refined.



- *Business Case Development*: Business cases help define a clear and purposeful solution based on well-defined and documented business needs. Having a business case helps to justify good projects, stop bad projects before they are started, and provides the basis for ongoing measurements after project completion to make sure that the business is getting the results they wanted.
- *Operational Planning*: In order to effect change on complex environments, it is necessary for organizations to develop operational plans. These plans minimize the risks associated with large technology deployments. Plans may incorporate key business processes and workflows, and help to identify any operational constraints.

Custom Development

Your organization requires solutions that meet you unique needs. CambridgeSoft consultants can assist with:

- *Custom Application Development*: Assess business needs, document specifications, and create custom web-based solutions for your enterprise.
- *Data Integration*: Create interfaces with other data management systems to incorporate your data into an enterprise system.
- *Installation and Customization*: Customize your solution to your specifications. Make certain that all technical and logistical installation processes are managed.

Deployment & Training

Develop a comprehensive road map for deployment of technology solutions across the enterprise. Our experts help you plan and deploy your solutions by:

- *Application Deployment*: Document, define and execute all of the actions required to support end user acceptance. Manage the deployment process to assure a smooth roll-out to the end-users
- *Beta and Pre-Release Programs*: Beta and pre-release programs involve a limited deployment to a small set of users in order to identify deployment readiness or logistical issues that must be addressed prior to a large-scale deployment. When early release programs are employed, the success rate of large scale deployments is greatly increased and end users are more likely to adopt the new technology.
- *Controlled Pilots*: Controlled pilots involve deploying a pre-production system to a small group of users to evaluate it's functional, usability, technical, and operational characteristics in a real-world environment prior to the completion of final system development. A controlled pilot helps identify and correct show-stopper technology or operational issues before a final roll out program is implemented.
- *Training*: Develop customized training materials for users, system administrators, and help desk personnel. If you choose to outsource training management, CambridgeSoft can schedule and conduct training for all users and stakeholders.

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CS Software Problem Report

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DETAILS OF THE PROBLEM

SYSTEM CONFIGURATION

SOFTWARE

Application Name _____

Version Number _____

Serial Number _____

SYSTEM

Windows (version) _____

MacOs (version) _____

Web Browser(s) (version) _____

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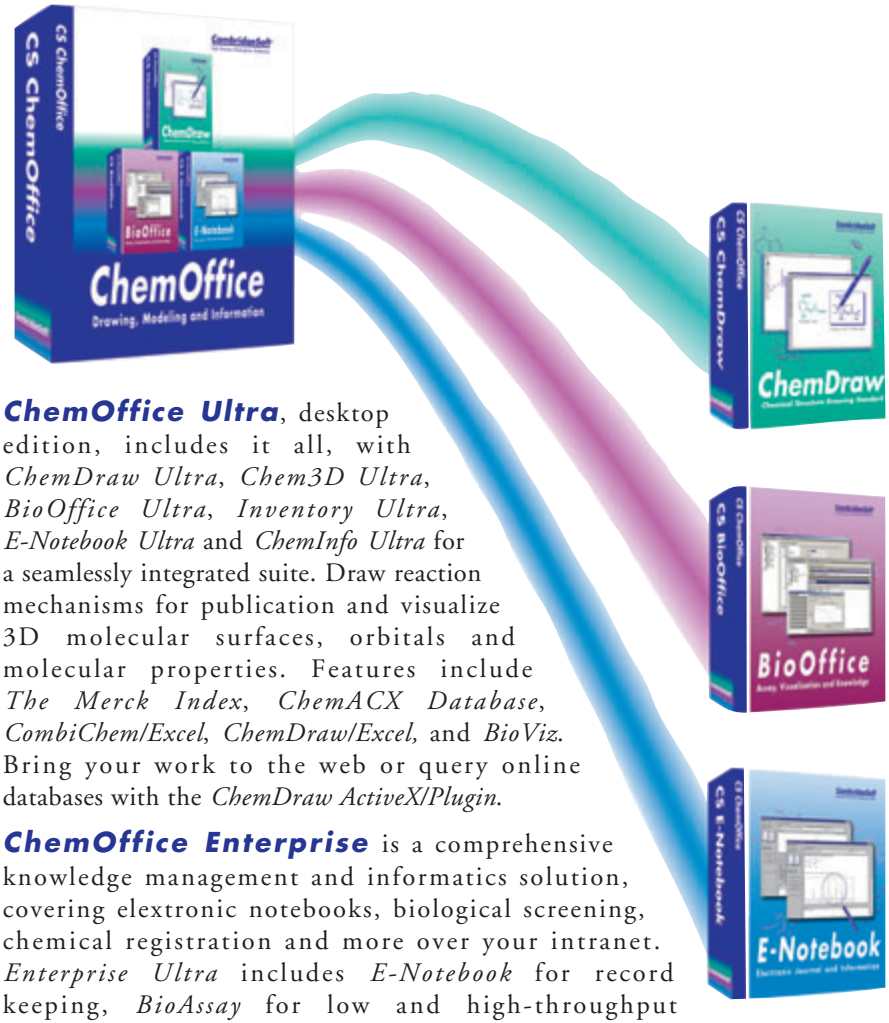
Desktop to Enterprise Solutions



ChemOffice Ultra, desktop edition, includes it all, with *ChemDraw Ultra*, *Chem3D Ultra*, *BioOffice Ultra*, *Inventory Ultra*, *E-Notebook Ultra* and *ChemInfo Ultra* for a seamlessly integrated suite. Draw reaction mechanisms for publication and visualize 3D molecular surfaces, orbitals and molecular properties. Features include *The Merck Index*, *ChemACX Database*, *CombiChem/Excel*, *ChemDraw/Excel,* and *BioViz*. Bring your work to the web or query online databases with the *ChemDraw ActiveX/Plugin*.

ChemOffice Enterprise is a comprehensive knowledge management and informatics solution, covering elextronic notebooks, biological screening, chemical registration and more over your intranet. *Enterprise Ultra* includes *E-Notebook* for record keeping, *BioAssay* for low and high-throughput screening, integrated plate inventory, *Inventory* for reagents, *BioSAR* for SAR reports, Registration system and *ChemACX Database* of available chemicals. Technologies include *ChemDraw ActiveX* and *Oracle Cartridge*.

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